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Ideal strength and ductility in metals from second and third-order elastic constants

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Under tensile loading the ideal strength of a solid is governed by mechanical instabilities corresponding to failure in tension or shear, indicative of intrinsically brittle or ductile behavior, respectively. Ideal-strength first-principles calculations are performed in this work on several hexagonal-close-packed (hcp) and body-centered-cubic (bcc) metals. It is shown that some metals fail in tension under uniaxial loading, whereas others fail in shear. The observed behavior is rationalized with a simple analytical model based on second-order and third-order elastic constants. This formalism correctly predicts the failure mode of all but one of the metals studied in this work and leads to fundamental new insights into why some classes of metals are intrinsically brittle or ductile. Further, for the transition metals, filling of the *d*-bands is shown to correlate with the type of mechanical instability encountered, thus providing new insights into the effect of alloying on the intrinsic mechanical behavior of hcp and bcc metals.

I. INTRODUCTION

For any given loading condition, the ideal strength of a crystalline solid forms an upper bound on the stress that the material can sustain prior to reaching a mechanical instability. The nature of the instability reached at this stress level can provide insights into the intrinsic failure mechanisms for a material. For example, under tensile loading crack initiation requires that the local normal stress perpendicular to the cleavage plane is equal to or larger than the ideal tensile strength[1–4]. However, when a material yields under tensile loading, it is possible for it to fail through a shear instability[5–9]. The tensile versus shear nature of the mechanical instability realized under tensile loading is of considerable interest as an indicator of whether a material will behave in an intrinsically brittle or ductile manner. For cubic metals, first-principles calculations of ideal strength under tensile loading have revealed shear instabilities for the ductile metals V and Nb, whereas more brittle materials such as W and Mo have been shown to fail in tension[6]. Similar studies in alloys[10–13] have been undertaken recently, yielding insights into the compositional effects on deformation behavior and ductility. For example, it has been shown that bcc-based Mo-alloys can be made intrinsically more ductile (less brittle) by tuning the *d* band filling through alloying[6].

Fundamentally, the occurence of any elastic instability under an external load depends on the variation of the deformed (or *apparent*) elastic constants with strain and the stress tensor acting on the material, as well as the magnitude and direction of the applied load. Along the load path, the various independent deformed elastic constants vary differently as a function of the imposed strain tensor and it is the detailed relations among them that determine the type of elastic instability that occurs.

Elastic instabilities can be calculated by employing Density Functional Theory (DFT), which has been a common approach in the literature[2,9,14–20]. In such studies, typically different amounts of strains are applied to a unit cell and at each strain the internal coordinates and lattice vectors perpendicular to the load are relaxed. In addition, the stress tensor and deformed elastic constants are calculated, from which elastic instabilities can be calculated. This approach however is computationally expensive due to the necessity to calculate deformed elastic constants at every imposed strain. In addition, it provides limited insight into the underlying mechanisms and physics that lead to elastic instabilities, resulting in intrinscially ductile or brittle behavior.

In this work, in addition to comparing to traditional ideal-strength calculations, an alternative approach is pursued to study ideal deformation behavior, elastic instabilities and intrinsic ductility. It is based on the observation that as a solid is deformed, its deformed elastic constants vary. Rather than performing a direct DFT calculation to obtain the deformed elastic constants, instead the deformed elastic constants are obtained as an expansion in terms of the applied strain tensor, involving the standard (undeformed) second-order elastic constants (SOEC's) and the third-order elastic constants (TOEC's). Via this approach, analytical expressions are obtained for the ideal failure type (shear vs. tensile), the failure strain and the failure stress. In addition, the variation of the deformed elastic constants with strain can be rationalized in terms of anharmonic effects, captured by the TOEC's. This formalism consequently leads to an enhanced fundamental understanding of the ideal deformation behavior and intrinsic ductility of solids in terms of the variation of deformed elastic constants and applied stress along a prescribed deformation path.

The formalism presented in the paper relies on knowledge of reliable SOEC's and TOEC's in particular. However, the accurate calculation of TOEC's is challenging due to their sensitivity to DFT parameters and strain range. To address this issue, a robust and general scheme is introduced to evaluate TOEC's from DFT calculations, which allows for a general way of estimating intrinsic deformation behavior of materials from basic elastic properties.

The outline of this paper is as follows. Sec. II presents the formalism and methods that are developed as part of this work. In particular, the Wallace formalism and elastic instabilities are reviewed in Section II A. Section II C describes the relation between deformed elastic constants, SOEC's, TOEC's and applied strains and Sec. II B describes a practical calculation scheme for TOEC's. The details of the DFT calculations used in this work are described in Sec. II D. Finally, Sec. III describes the results and discussion. Some of the detailed derivations of the equations derived in this work are rather lengthy and are presented in full in the Appendix.

II. METHODOLOGY

A. Wallace formalism and elastic instabilities

The elastic stability of a solid under zero stress is governed by the eigenvalues of its elastic-constant tensor; specifically, all 6 eigenvalues of this tensor must be larger than zero for the solid to be elastically stable. A generalization of this concept was introduced by Wallace to consider the elastic stability of solids under stress[21]. In such cases, elastic stability is governed by the Wallace tensor, defined as follows:

$$B_{ijkl} = C'_{ijkl} + \frac{1}{2}\left(\sigma_{il}\delta_{jk} + \sigma_{jl}\delta_{ik} + \sigma_{ik}\delta_{jl} + \sigma_{jk}\delta_{il} - 2\sigma_{ij}\delta_{kl}\right) \quad (1)$$

where the term C'_{ijkl} represents the elastic constants in the deformed configuration[17,21,22], σ_{ij} denotes the applied stress acting on the solid, and δ_{ij} is the Kronecker-delta. Note that the Wallace tensor reduces to the standard (undeformed) SOEC's for a solid under zero stress. The eigenvalues of the symmetrized Wallace tensor govern the elastic stability of a solid under stress[23]. In the present context, the symmetrized Wallace tensor, $\bar{\boldsymbol{B}}$ is defined as $\bar{\boldsymbol{B}} = 1/2\ (\boldsymbol{B} + \boldsymbol{B}^T)$ (with $\boldsymbol{B}$ given in Eq. 1), where the use of Voigt notation is implied so that both $\boldsymbol{B}$ and $\bar{\boldsymbol{B}}$ reduce to 6×6 matrices. In the remainder of this paper, the Wallace-tensor B_{ijkl} refers to the *symmetrized* Wallace tensor. We will consider cubic and hexagonal crystals in the remainder of this work, although the same formalism may be readily applied to lower-symmetry materials.

The terms C'_{ijkl} and σ in Eq. 1 can be evaluated directly from DFT calculations for every strain along a deformation path, after which the eigenvalues and eigenvectors of the Wallace tensor can be obtained to study elastic instabilties. In this work elastic instabilities are studied by computing the Wallace tensor (Eq. 1) as a function of strain via higher-order elastic constants. A similar approach has been used in the past to study a small set of cubic materials and metallic glasses[4,24]. The deformed elastic constants C'_{ijkl} and the stress σ are calculated as described in subsequent sections, from a knowledge of the SOEC's, TOEC's and applied strain only.

Consider a uniaxial loading condition for a hexagonal or cubic crystal. The load is applied along the [001] axis for the cubic material and along the [0001] axis for the hexagonal material, both generically referred to as the c axis in this paper. For this loading condition, with a Green-Lagrange strain ξ along the c axis, the Cauchy stress tensor σ may be computed according to formalism outlined in the Appendix. In particular, Eqs. A1 - A9 detail the calculation of the strain energy density in terms of SOEC's and TOEC's and the general calculation of the stress tensor with strain. Further, the Piola-Kirchhoff stress tensor is obtained from the SOEC's, TOEC's and the imposed strain ξ along c (allowing for Poisson contraction perpendicular to c). The derivation is somewhat lengthy and is presented in the Appendix: Eqs. A10 - A15 for cubic crystals and Eqs. A16 - A20 for hexagonal crystals.

The general derivation of the Wallace tensors starts with Eq. 1 and then follows the lines of Eqs. B1 - B6 in the Appendix. In particular, Eqs. B7 and B8 in the Appendix detail the Wallace tensor for cubic and hexagonal crystals under c-loading, respectively. This formalism allows one to analytically calculate the ideal deformation behavior of materials based on just a knowledge of the SOEC's and TOEC's. The formalism pertaining to TOEC's and their calculation is discussed in subsequent sections.

B. Calculations of second-order and higher-order elastic constants

The formalism outlined in Sec. II A requires the knowledge of SOEC's and TOEC's, which are used to calculate stresses and deformed elastic constants as a function of strain. This section outlines the details of those calculations.

The third-order elastic constants are defined as

$$C_{ijklmn} = \rho_0 \frac{\partial^3 F}{\partial\eta_{ij}\partial\eta_{kl}\partial\eta_{mn}}|_{\eta=0}, \quad (2)$$

where F is the Helmholtz free energy density (per unit

mass), η_{ij}, the Green-Lagrange strain, and ρ_0, the density of the undeformed state. It should be noted that the formalism considered in this paper is only being applied to SOEC's and TOEC's calculated at absolute zero temperature using DFT, hence the Helmholtz free energy is identical to the total energy E, $F = E$.

If the TOECs contain minor and major symmetries and thus can be written in Voigt notation, but no point symmetry other than the identity, the sixth-order elastic tensor will consist of 56 unique constants. These can be evaluated efficiently using a 9-point finite difference stencil, employing a maximum strain of $\eta_{max} = 0.05$ for both tension and compression. The value $\eta_{max} = 0.05$ was chosen after extensive convergence testing and is located near a local plateau of the TOECs as a function of strain[25,26]. In general, both the SOEC's and TOEC's obtained from DFT do not precisely obey the desired symmetry dictated by the underlying crystal point group[18,27–31]. The correct symmetry is therefore restored by performing an average over the pertinent point group operations. This method is described in detail in the Appendix.

C. Deformed elastic constants and stress tensor

The calculation of the Wallace tensor requires the deformed elastic constants on one hand and the stress tensor acting on the structure on the other hand. Eqs. 3 denote the deformed elastic constants for cubic crystals under c-loading. Eqs. 4 denote the deformed elastic constants for hexagonal crystals under c-loading.

$$C'_{11} = C_{11} + \eta(3C_{11} + C_{111} + C_{112} + C_{12}) + \xi(-C_{11} + C_{112} + C_{12}), \tag{3a}$$
$$C'_{12} = C_{12} + 2\eta(C_{112} + C_{12}) + \xi(C_{123} - C_{12}), \tag{3b}$$
$$C'_{13} = C_{12} + \eta(C_{112} + C_{123}) + \xi(C_{112} + C_{12}), \tag{3c}$$
$$C'_{33} = C_{11} + 2\eta(-C_{11} + C_{112} + 2C_{12}) + \xi(4C_{11} + C_{111}), \tag{3d}$$
$$C'_{44} = C_{44} + \eta\left(\frac{1}{4}C_{11} + \frac{3}{4}C_{12} + C_{144} + C_{166}\right) + \xi\left(\frac{1}{4}C_{11} + \frac{1}{4}C_{12} + C_{166} + C_{44}\right), \tag{3e}$$
$$C'_{66} = C_{66} + \eta\left(2C_{166} + \frac{1}{2}C_{11} + \frac{1}{2}C_{12} + 2C_{66}\right) + \xi\left(-C_{66} + \frac{1}{2}C_{12} + C_{144}\right) \tag{3f}$$

$$C'_{11} = C_{11} + \eta(3C_{11} + C_{12} + C_{111} + C_{112}) + \xi(-C_{11} + C_{113} + C_{13}), \tag{4a}$$
$$C'_{12} = C_{12} + \eta(2C_{12} + \frac{5}{3}C_{112} + \frac{1}{3}C_{111} - \frac{4}{3}C_{166}) + \xi(-C_{12} + C_{123}), \tag{4b}$$
$$C'_{13} = C_{13} + \eta(C_{123} + C_{113}) + \xi(C_{13} + C_{133}), \tag{4c}$$
$$C'_{33} = C_{33} + \eta(2C_{13} - 2C_{33} + 2C_{133}) + \xi(4C_{33} + C_{333}), \tag{4d}$$
$$C'_{44} = C_{44} + \eta\left(\frac{1}{4}C_{11} + \frac{1}{4}C_{12} + \frac{1}{2}C_{13} + C_{144} + C_{155}\right) + \xi\left(C_{44} + C_{355} + \frac{1}{4}C_{33} + \frac{1}{4}C_{13}\right), \tag{4e}$$
$$C'_{66} = \frac{1}{2}\left(C'_{11} - C'_{12}\right) \tag{4f}$$

In Eqs. 3 and 4, ξ is the strain along c and $\eta = \eta_1 = \eta_2$ is the strain in the a-b plane, perpendicular to the c-direction. The terms C_{ij} represent the standard second-order elastic constants (SOEC's) in the undeformed configuration and the terms C_{ijk} represent the third-order elastic constants (TOEC's) in the undeformed configuration. The load cases considered in this work are uniaxial along c, which implies that ξ and η are not independent. This corresponds physically to a situation in which a load is applied along c and all other crystal directions are allowed to relax to zero stress (e.g. Poisson contraction). In fact for this load case we can express $\eta = \eta\left(\xi, C_{ij}, C_{ijk}\right)$. Consequently, η in Eqs. 3 and 4 can be eliminated so that the deformed elastic constants can be expressed as only functions of the SOEC's, TOEC's and ξ.

The detailed derivations pertaining to the calculations of TOEC's and the deformed elastic constants are rather lengthy and are presented in full in the Appendix. It

should be noted that the choice for TOEC's is not unique in e.g. Eqs. 4 and combinations of other TOEC's could be used instead of those. For the case of hcp materials, Eqs. 5 describe some of these relations between TOEC's. A complete overview is presented in Eqs. C13.

$$C'_{111} = C_{222} - C_{661} + C_{662}, \tag{5a}$$
$$C'_{112} = C_{222} - 2C_{661} - 2C_{662}, \tag{5b}$$
$$C'_{123} = C_{223} - 2C_{366} \tag{5c}$$

D. DFT calculations

For the elemental metals all calculations were performed using the Vienna Ab Initio Simulation Package (VASP)[32,33]. In these calculations use was made of the Perdew-Burke-Ernzerhof generalized gradient functional (PBE-GGA)[34], and the projector augmented wave (PAW) method[35,36]. An energy cutoff for the plane waves of 700 eV was used, and smearing of the electronic occupancies was performed using the Methfessel-Paxton scheme[37], with a broadening of 0.05 eV. Integrations in the Brillouin zone were carried out using Monkhorst-Pack k-point sampling[38] with a density chosen such that the number of k-points in the first Brillouin zone times the number of atoms in the cell equals approximately 30,000-40,000. The employed PAW potentials for Sc, Ti, Y, Zr and Hf include s and p semi-core states as valence electrons. For the other elements, only the outermost s- and d-states are used as valence. The maximum calculated tensile stress σ_{33} that occurs along the deformation path (similar to the ultimate tensile strength) is converged to within approximately 2% with these DFT settings.

III. RESULTS AND DISCUSSION

In this section, the ideal deformation behaviors of 4 bcc metals (Mo, Nb, W and Ta) and 13 hcp metals (Be, Mg, Os, Re, Ru, Ti, Y, Zn, Zr, Co, Tc, Sc and Hf) are studied. Lattice stabilities are calculated as a function of the strain ξ along the c axis, and the failure modes are determined, employing only the SOEC's and TOEC's. This results in a categorization of the elemental metals into two classes: those that fail in shear (intrinsically ductile) or in tension (intrinsically brittle) for this loading condition.

A. Elastic instabilities and intrinsic ductility

Previously established relations between atomistic (ideal) measures of ideal deformation behavior and true (experimental) deformation behavior allow us to compare the results obtained in this work to experimental findings in the literature[39]. A direct comparison between experimental and theoretical measures of ductility is not straight-forward because elongation and reduction of area depend critically on several factors, including temperature, grain size, processing route (e.g. annealed vs as-fabricated), impurity concentrations, and strain rate. However, keeping these factors constant as much as possible across various metals and alloys allows for a qualitative comparison to be made. Table I shows experimentally reported values of elongation for several commericially pure metals subject to tension together with computed ideal failure mode. Tables II and III show the calculated elastic properties and failure modes for the cubic and hcp metals considered in this work, respectively.

Turning first to the cubic metals studied in this work, it is found that Mo and W are intrinsically brittle whereas Nb and Ta exhibit intrinsically ductile behavior. This is consistent with i) experimental investigations which show that Nb and Ta dogbone samples have significantly higher elongations to fracture in tensile tests than Mo and W, respectively[40–43] and ii) evidence of a significantly higher ductile-to-brittle-transition temperature in Mo and W compared to Nb and Ta[44–48]. Table I shows an interesting trend, namely commercially pure W and Mo having significantly less tensile elongation (1-5 % and 10-15 %, respectively) than Ta and Nb (70 % and 50 %, respectively). This corroborates the findings in this work that Nb and Ta are intrinsically ductile and exhibit ideal shear failure whereas Mo and W are intrinscially brittle and fail in tension. These results are further consistent with previous computational studies in which direct ideal-strength calculations were performed on several bcc metals[8,49–51]. Interestingly, Mo & W and Nb & Ta are from the same columns in the periodic table, underlining the role of d-band filling in establishing the detailed deformation mechanisms of transition metals[6].

Table III shows the calculated SOEC's, TOEC's and failure modes and strains for several transition metals with the hcp structure, in addition to the non-transition metals Be and Mg. For comparison, deformation properties for these metals are calculated i) by the formalism developed in this work using SOEC's and TOEC's and ii) by explicit DFT calculations of the Wallace tensor and elastic constants along the strain path. The following 5 metals are found to fail in tension: Be, Mg, Os, Re, Ru, whereas the following 8 fail in a ductile shear mode: Ti, Y, Zn, Zr, Co, Tc, Sc, Hf. Table I shows a compilation of reported experimental elongations at break for high purity ($\geq$ 99.98%) metals at room temperature. Not all metals considered in this work are included, but only those for which reliable and consistently measured data could be found.

With the exception of Re, the metals that are predicted computationally to be intrinsically ductile exhibit the largest elongations ranging from 15-72 %. On the

other hand, the metals predicted to be intrinsically brittle show elongations in the range 1-15 %, again with the exception of Re. Although this anomalous behavior of Re with predicted tensile failure but experimentally measured high elongations is not fully understood, it is known from previous work that Re has a strong propensity for deformation twinning, which may help explain its high degree of measured plasticity[52,53].

It is found that the hcp metals from groups III and IV (Sc, Y, Ti, Zr, Hf) fail in shear whereas those from group VIII (Ru and Os) fail in a brittle tensile mode. The formalism further shows that Tc fails in shear, whereas Re fails in tension, despite these metals both being from group VII and thus having the same *d*-band filling. We note however, that the failure strains for tension and shear for Re are very close (to within 1 %) and hence, although Re fails in tension according to the formalism, it is on the verge of shear failure. In fact, the difference is likely within the error bars of the SOEC's, TOEC's and DFT calculations. These results suggest that *d*-band filling is a descriptor for rationalizing the mechanical behavior across the transition metals for both cubic and hcp materials.

The failure strains in the *c*-direction according to the analytical model and direct DFT calculations are also shown in Table III for the hcp metals. It can be seen that the agreement is reasonable with typical discrepancies ranging from 1 to 5 percent. This is excellent agreement, given the simplicity of the model that relies only on elastic constants and given the technical difficulties in robustly calculating TOEC's. We find that the precise failure strain is rather sensitive to small changes in the TOEC's, however the type of failure mode (shear vs. tension) can be calculated rather robustly. The agreement shown in Table III between the analytical model and direct DFT calculations indicates that the use of non-linear elasticity is a viable method for calculating ideal deformation behavior.

B. Origins of shear and tensile failure

The failure mode of cubic and hcp materials under loading along c is determined by a complex combination of SOEC's and TOEC's. For cubic materials, the eigenvalues of the Wallace tensor associated with shear failures are given as C'_{66}, $C'_{11}-C'_{12}$ and $C'_{44}+\frac{\sigma_{33}}{2}$. In turn, these quantitities depend on the (undeformed) SOEC's, the TOEC's, η and ξ as described by Eqs. 3 (a)-(f). ξ and η are related to each other by a rather complicated function of SOEC's and TOEC's, but for most materials this relation can be approximated for small strains by the Poisson ratio ν, i.e. $-\frac{\eta}{\xi}\approx\nu\approx 0.30$.

Referring to Eq. 3 (f) for C'_{66}, it is seen that intrinsically ductile behavior is favored by cubic materials that have (i) low values for $C_{44}=C_{55}=C_{66}$, (ii) large (negative) values for C_{166} and large (negative) values for the TOEC C_{144}. For the eigenvalue $C'_{11}-C'_{12}$ similar observations hold, with (i) a small (absolute value) for $C_{11}-C_{12}$ favoring shear failure, along with (ii) a large negative value for C_{112}. Brittle tensile failure on the other hand is associated with more complicated eigenvalues (not shown here) and is favored by materials with (i) large values for (undeformed elastic constants) $C_{11}=C_{33}$, and (ii) a large (negative) TOEC C_{111}.

For hcp metals, the expressions for the eigenvalues of the Wallace tensor are more complicated, but a similar rationale holds true as for cubic materials. During loading, the eigenvalues of the Wallace tensor vary as a function of the imposed strain ξ, with the SOEC's and TOEC's dictating the rate of decay of each eigenvalue with strain. In general, brittle behavior is favored for materials with relatively low values for C_{33} and TOEC's that result in relatively high softening of C_{33} with strain along c. Eq. 4 (d) shows that a large negative value of C_{333} in particular favors brittle behavior. In addition, brittle behavior is favored for material with high shear moduli (C_{44} , C_{55}, C_{66}) and TOEC's that lead to a low softening of the shear moduli with strain. It is the delicate balance between these SOEC's and TOEC's that determines the ultimate failure mechanism. For example, the hcp metals Os and Ru have high moduli C_{33} (818 and 636 GPa, respectively) but nonetheless fail in tension along c since the TOEC C_{333} is a large negative number and in addition the shear moduli C_{44} are high (255 and 184 GPa, respectively). Further, the TOEC's governing the softening of the shear moduli with strain such as C_{366} are moderate in magnitude, which avoids hitting a shear instability in these materials. Ductile materials such as Nb on the other hand have low (undeformed) shear moduli (C_{44} , C_{55}, C_{66}) which already brings the material under zero load near a shear instability. Loading along c decreases this modulus further and - in conjunction with the other SOEC's, TOEC's and the applied stress - leads to a quick shear failure after a small amount of strain.

This view on failure mechanisms fits into the formalism developed by Pugh[58], which states that the ratio of bulk (K) to shear (G) modulus, K/G, is a measure of intrinsic ductility. Pugh's ratio can be rationalized to some extent. The ratio relates the competition between brittle failure and shear failure in the material. For an isotropic material it is supposed that the tendency for shear failure varies inversely with G, while the tendency for brittle failure should vary inversely with the elastic constant, C_{11}, for a material with a tensile load applied along $\langle 100\rangle$. This ratio written in terms of K and G is $\frac{C_{11}}{G}=\frac{K}{G}+\frac{4}{3}$. However, it should be noted that Pugh's ratio does not include any notion of higher-order elasticity, i.e. it does not consider the softening of the various elastic moduli with strain.

TABLE I. Experimentally reported values of elongation for several commericially pure metals subject to tension[54–57], together with computed ideal failure mode.

Metal	Elongation (%)	Failure mode
Titanium	40-72	Shear
Zirconium	35-40	Shear
Hafnium	35-43	Shear
Niobium	50	Shear
Tungsten	1-5	Tension
Tantalum	70	Shear
Molybdenum	10-15	Tension
Rhenium	25-28	Tension
Magnesium	2-15	Tension
Beryllium	1-5	Tension

TABLE II. Calculated SOEC's, TOEC's and ideal-failure characteristics for selected cubic metals and intermetallics. Failure modes are characterized as either shear (S) or tension (T).

	Mo	Nb	W	Ta
SOEC's (GPa)				
C_{11}	462	265	516	271
C_{12}	171	126	215	168
C_{44}	85	25	134	71
TOEC's (GPa)				
C_{111}	-4688	-1812	-5613	-2567
C_{112}	-974	-233	-967	-1116
C_{123}	-37	-1221	-420	1024
C_{144}	-447	-540	-848	-298
C_{155}	-756	11	-816	-625
C_{456}	-176	207	-571	40
Failure characteristics				
Failure mode	T	S	T	S

TABLE III. Calculated SOEC's, TOEC's and ideal-failure characteristics for 13 hcp metals. Failure modes are characterized as either shear (S) or tension (T).

	Be	Mg	Os	Re	Ru	Ti	Y	Zn	Zr	Co	Tc	Sc	Hf
SOEC's (GPa)													
C_{11}	333	65	724	626	567	178	79	156	148	346	500	101	188
C_{12}	16	21	237	270	179	88	26	56	68	126	222	37	75
C_{23}	5	23	228	219	170	84	20	44	70	122	186	28	74
C_{33}	392	62	818	682	636	189	82	68	164	359	553	102	200
C_{44}	171	19	255	163	184	42	26	42	27	62	135	31	54
TOEC's (GPa)													
C_{222}	-2845	-809	-9395	-7746	-6690	-1725	-670	-3676	-1087	-4437	-5703	-852	-1767
C_{166}	116	-104	-1992	-1364	-1156	-364	-163	-809	-267	-858	-1142	-204	-355
C_{266}	-2132	-274	-1802	-1973	-1744	-341	-129	-429	-243	-1029	-1000	-185	-442
C_{223}	707	187	-105	227	-461	61	-43	976	-64	-219	-978	-82	11
C_{366}	397	65	-225	356	-203	-224	-120	141	-231	31	-682	-107	-246
C_{233}	-838	-438	-3501	-2514	-2042	-607	-143	-2215	-317	-1191	-1555	-165	-436
C_{333}	-2048	60	-5674	-4609	-5476	-876	-526	5489	-1239	-3478	-5325	-711	-1397
C_{155}	-475	-105	-1912	-1128	-1281	-341	-82	-169	-151	-498	-1108	-122	-341
C_{255}	-435	-91	-606	-809	-529	12	-50	-186	132	-261	-1039	-81	5
C_{355}	-489	-103	-1500	-847	-1134	-96	-124	-134	-66	-644	-1607	-163	-156
Failure characteristics													
$\bar{\xi}$ (direct DFT)	0.13	0.22	0.15	0.19	0.15	0.24	0.20	0.12	0.16	0.15	0.18	0.22	0.14
$\bar{\xi}$ (analytical)	0.17	0.25	0.19	0.23	0.19	0.27	0.27	0.13	0.13	0.17	0.23	0.27	0.16
Failure mode	T	T	T	T	T	S	S	S	S	S	S	S	S

IV. SUMMARY AND CONCLUSIONS

A formalism is developed in this work to study the ideal deformation behavior of single-crystal hcp and bcc solids. This formalism can be used to compute failure modes of materials and is a function only of elastic constants and applied strain, in particular SOEC's and TOEC's. It accounts for the anharmonicity of elastic constants as a function of strain and employs the Wallace tensor, its eigenvalues and eigenvalues to characterize the failure mode of materials. In order to apply this formalism, a practical and robust way of calculating SOEC's and in particular TOEC's is developed and described in this work.

The formalism is applied in this paper to 4 bcc transition metals (Nb, Ta, Mo and W) and 13 hcp metals (Be, Mg, Os, Re, Ru, Ti, Y, Zn, Zr, Co, Tc, Sc and Hf). It is found that Nb and Ta fail in shear and are consequently intrinsically ductile whereas Mo and W fail in tension and are intrinsically brittle. Among the hcp metals, Mg, Be, Os, Ru and Re are found to be intrinsically brittle, whereas Ti, Y, Zn, Zr, Co, Tc, Sc and Hf are intrinsically ductile. Re is a special case in which the shear and tensile failure modes occur near the same strain along c, and hence the precise failure mechanism cannot easily be determined. The formalism predicts W, Mo, Be, Mg, Re and Os to be brittle, separating those metals from more ductile metals such as Hf, Sc and Ti. Based on available experimental data on several commerically-pure transition metals, their appears to exist an excellent correlation between intrinsic ductility and tensile elongation.

It is further found that d-band filling appears to be an important physical parameter in determining the deformation behavior of transition metals (and alloys). Metals from groups III and IV with the hcp structure (Sc, Y, Ti, Zr, Hf) fail in shear whereas those from group VIII (Ru and Os) fail in a brittle tensile mode. Further, cubic metals from group V fail in shear whereas those in group VI fail in tension. This formalism provides new insights into the origins of these differences in failure modes and relates it to basic elastic properties, in particular the SOEC's and the degree to which the SOEC's soften under strain, which is described by the TOEC's. Metals with relatively high shear moduli tend to exhibit intrinsically brittle behavior, consistent with Pugh's formalism, however this is merely a rule of thumb and the detailed answer depends on a complicated trade-off between the SOEC's and TOEC's as discussed in this paper. Metals with relatively low shear moduli on the other hand tend to fail in shear, in particular if the shear modulus softens significantly with an increase in the applied strain.

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Appendix A: Strain energy density: formalism and results

1. General expressions

Consider the mapping between the reference and current configuration of a continuum solid. In the reference configuration, a particle occupies a point $\boldsymbol{p}$ with spatial coordinates $\boldsymbol{X} = X_1\boldsymbol{e}_1 + X_2\boldsymbol{e}_2 + X_3\boldsymbol{e}_3$, where e_1, e_2, e_3 is a Cartesian reference triad and X_1, X_2, X_3 are the reference coordinates. Upon deformation of the body, the point originally at $\boldsymbol{X}$ is translated by the displacement vector $\boldsymbol{u}(X_1, X_2, X_3)$ to its final coordinates $\boldsymbol{x}(X_1, X_2, X_3)$, see Eq. A1 .

$$\boldsymbol{x}(X_1, X_2, X_3) = \boldsymbol{u}(X_1, X_2, X_3) + \boldsymbol{X}(X_1, X_2, X_3) \quad \text{(A1)}$$

Based on this description, a deformation gradient is formulated as in Eq. A2. The Green-Lagrangianstrain tensor $\boldsymbol{\eta}$ then follows from $\boldsymbol{F}$ as shown in Eq. A3, where $\boldsymbol{I}$ denotes the identity matrix.

$$\boldsymbol{F} = \frac{\partial x_i}{\partial X_j} \quad \text{(A2)}$$

$$\boldsymbol{\eta} = \frac{1}{2}\left(\boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I}\right) \quad \text{(A3)}$$

With the notation now established, the strain energy density E (per unit mass) can be expanded in terms of the second-order elastic constants (SOEC's), C_{ij}, third-order elastic constants (TOEC's), C_{ijk}, and the Green-Lagrangianstrain, $\boldsymbol{\eta}$, as in Eq. A4, where ρ_0 represents the mass density in the undeformed state and the terms η_i represent the components of the tensor defined in Eq. A3. The symmetry of the SOEC's and TOEC's will be applied in the expansions, which simplifies the resulting expressions considerably. Note that in Eq. A4, the Voigt notation $\eta_{11} \mapsto \eta_1$, $\eta_{22} \mapsto \eta_2$, $\eta_{33} \mapsto \eta_3$, $\eta_{23} \mapsto \eta_4/2$, $\eta_{13} \mapsto \eta_5/2$, $\eta_{12} \mapsto \eta_6/2$ has been applied.

$$\rho_0 E(\boldsymbol{\eta}) = \frac{1}{2!}\sum_{i,j=1}^{6} C_{ij}\eta_i\eta_j + \frac{1}{3!}\sum_{i,j,k=1}^{6} C_{ijk}\eta_i\eta_j\eta_k + \dots \quad \text{(A4)}$$

In this work, strain control is assumed and the crystals are loaded uniaxially along the c-axis. All other degrees of freedom are allowed to relax to zero stress by means of Poisson contraction. The imposed strain components along c is denoted by ξ in this work and the resulting equilibrium strain along the a and b directions is $\eta_1 = \eta_2 = \bar{\eta}$. The deformation gradient $\boldsymbol{F}$ and the corresponding Green-Lagrangianstrain tensor $\boldsymbol{\eta}$ that pertain to this loading situation are presented in Eqs. A5 and A6.

$$\boldsymbol{F} = \begin{bmatrix} \sqrt{2\bar{\eta}+1} & 0 & 0 \\ 0 & \sqrt{2\bar{\eta}+1} & 0 \\ 0 & 0 & \sqrt{2\xi+1} \end{bmatrix} \tag{A5}$$

$$\boldsymbol{\eta} = \begin{bmatrix} \bar{\eta} & 0 & 0 \\ 0 & \bar{\eta} & 0 \\ 0 & 0 & \xi \end{bmatrix} \tag{A6}$$

Further, we introduce the different measured of stress that are used throughout this work. First, the second Piola-Kirchhoff stress tensor $\mathbf{S}$ is defined in Eq. A7 as a derivative of the strain energy density w.r.t. to Green-Lagrangian strains.

$$\mathbf{S}_{ij} = \rho_0 \frac{E}{\eta_{ij}} \tag{A7}$$

Nanson's equation is used to convert between $\mathbf{S}$ and the Cauchy stress tensor σ according to Eq. A8, where $|\mathbf{F}|$ denotes the determinant of $\mathbf{F}$.

$$\mathbf{S} = |\mathbf{F}|\,\mathbf{F}^{-1}\sigma\mathbf{F}^{-T} \leftrightarrow \boldsymbol{\sigma} = \frac{1}{|\mathbf{F}|}\mathbf{F}\mathbf{S}\mathbf{F}^{T} \tag{A8}$$

For a loading direction where only σ_{33} (and S_{33}) are nonzero, and $\mathbf{F}$ given by Eq. A5, the relation between σ_{33} and S_{33} is particularly simple, see Eq. A9.

$$\sigma_{33} = \frac{\sqrt{2\xi+1}}{2\bar{\eta}+1} S_{33} \tag{A9}$$

In the next sections, we derive explicit relations between strain, stress and elastic constants for cubic and hexagonal crystals under a uniaxial stress along c.

2. Cubic crystal system

We consider a cubic material that is loaded along the c-axis by a Green-Lagrangian strain denoted by ξ. Initially, we allow for additional strains denoted by $\eta_1, \eta_2, \eta_4, \eta_5, \eta_6$. Consider an expansion of the strain energy density up to and including SOEC's. When the symmetry of the SOEC's is invoked, the expression in Eq. A10 is obtained.

$$\rho_0 E(\boldsymbol{\eta}) = C_{11}\frac{\eta_1^2}{2} + C_{11}\frac{\eta_2^2}{2} + C_{33}\frac{\xi^2}{2} + C_{44}\frac{\eta_4^2}{2} + C_{44}\frac{\eta_5^2}{2} + C_{44}\frac{\eta_6^2}{2} + C_{12}\eta_1\eta_2 + C_{12}\xi\eta_2 + C_{12}\eta_1\xi \tag{A10}$$

Eq. A10 generally suffices for small strains. For larger strains, a higher-order expansion of the strain energy density involving TOEC's is required, as shown in Eq. A11, where the terms P_i are given in Eqs. A12.

$$\rho_0 E(\boldsymbol{\eta}) = C_{11}P_{1c} + C_{44}P_{2c} + C_{12}P_{3c} + C_{111}P_{4c} + C_{112}P_{5c} + C_{123}P_{6c} + C_{144}P_{7c} + C_{155}P_{8c} + C_{456}P_{9c} \tag{A11}$$

$$P_{1c} = \frac{\eta_1^2}{2} + \frac{\eta_2^2}{2} + \frac{\xi^2}{2}, \tag{A12a}$$

$$P_{2c} = \frac{\eta_4^2}{2} + \frac{\eta_5^2}{2} + \frac{\eta_6^2}{2}, \tag{A12b}$$

$$P_{3c} = \eta_1\eta_2 + \eta_2\xi + \eta_1\xi, \tag{A12c}$$

$$P_{4c} = \frac{1}{6}\left(\eta_1^3 + \eta_2^3 + \xi^3\right), \tag{A12d}$$

$$P_{5c} = \frac{1}{2}\left(\eta_2\eta_1^2 + \xi\eta_1^2 + \eta_2^2\eta_1 + \xi^2\eta_1 + \eta_2\xi^2 + \eta_2^2\xi\right), \tag{A12e}$$

$$P_{6c} = \eta_1\eta_2\xi, \tag{A12f}$$

$$P_{7c} = \frac{1}{2}\left(\eta_1\eta_4^2 + \eta_2\eta_5^2 + \xi\eta_6^2\right), \tag{A12g}$$

$$P_{8c} = \frac{1}{2}\left(\eta_2\eta_4^2 + \xi\eta_4^2 + \eta_1\eta_5^2 + \xi\eta_5^2 + \eta_1\eta_6^2 + \eta_2\eta_6^2\right), \tag{A12h}$$

$$P_{9c} = \eta_4\eta_5\eta_6 \tag{A12i}$$

In this work, we consider deformations of the type shown in Eq. A5, resulting in a strain tensor as shown in Eq. A6. This implies that $\eta_4 = \eta_5 = \eta_6 = 0$ and also $\eta_1 = \eta_2$. If we further invoke that $\eta_1 = \eta_2 = \bar{\eta}$ and $\eta_3 = \xi$, Eq. A13 is obtained.

$$\rho_0 E(\boldsymbol{\eta}) = \left(\frac{C_{111}}{3} + C_{112}\right)\bar{\eta}^3 + \left(C_{11} + C_{12} + C_{112}\xi + C_{123}\xi\right)\bar{\eta}^2 + \left(C_{112}\xi^2 + 2C_{12}\xi\right)\bar{\eta} + \frac{C_{111}\xi^3}{6} + \frac{C_{11}\xi^2}{2} \tag{A13}$$

The strains $\bar{\eta}$ and ξ are clearly not independent and in fact, we can write $\bar{\eta} = \bar{\eta}(\xi)$.The value of $\bar{\eta}$ can be obtained by differentiating Eq. A13 with respect to $\bar{\eta}$ and setting the resulting expression equal to zero. The governing quadratic equation in $\bar{\eta}$ is shown in Eq. A14. The resulting expression for $\bar{\eta}$ is rather long and is not shown here.

$$3\left(\frac{C_{111}}{3} + C_{112}\right)\bar{\eta}^2 + 2\left(C_{11} + C_{12} + C_{112}\xi + C_{123}\xi\right)\bar{\eta} + 2C_{12}\xi + C_{112}\xi^2 = 0 \Rightarrow \bar{\eta} = \bar{\eta}(\xi) \tag{A14}$$

The component S_{33} of the second Piola-Kirchhoff stress tensor can be obtained from Eq. A7 (upon the insertion of $\bar{\eta}$ and ξ) and is shown in Eq. A15. All other components in $\mathbf{S}$ are zero and the same is true for σ.

$$S_{33} = \left(2C_{12} + 2C_{112}\xi\right)\bar{\eta} + C_{11}\xi + \left(C_{112} + C_{123}\xi\right)\bar{\eta}^2 + \frac{C_{111}\xi^2}{2} \tag{A15}$$

The Cauchy stress component σ_{33} can now be obtained for every strain ξ as follows.

1. Consider an applied strain ξ
2. Compute the resulting strain (Poisson contraction) $\bar{\eta}$ from Eq. A14
3. Compute S_{33} from Eq. A15
4. Compute σ_{33} from Eq. A9

3. Hexagonal crystal system

For the hexagonal crystal system, the formalism follows a similar path as for the cubic crystal system. The various expressions are longer however, due to the lower amount of symmetry present.

Consider an imposed strain ξ along the c-axis of a hexagonal material, in addition to strains denoted by $\eta_1, \eta_2, \eta_4, \eta_5, \eta_6$. Consider first the expansion of Eq. A4, retaining only terms up to and including the SOEC's (hence, ignoring the TOEC's for now). This gives the energy expression in Eq. A16, in which the symmetry of the SOEC's has been applied.

$$\rho_0 E\left(\boldsymbol{\eta}\right) = C_{11}\frac{\eta_1^2}{2} + C_{11}\frac{\eta_2^2}{2} + C_{33}\frac{\xi^2}{2} + C_{44}\frac{\eta_4^2}{2} + C_{44}\frac{\eta_5^2}{2} + \frac{1}{2}\left(C_{11} - C_{12}\right)\frac{\eta_6^2}{2} + C_{12}\eta_1\eta_2 + C_{13}\eta_1\xi + C_{13}\eta_2\xi \tag{A16}$$

For large strains, the expansion in Eq. A16 is not sufficient and instead, TOEC's have to be included as well. The expansion of the strain energy up to the third order in strain is given in Eq. A17, in which the terms P are given in Eq. A18. Note that in Eq. A17, the symmetry of the SOEC's and TOEC's has been incorporated to simplify the resulting expression.

$$\begin{aligned}\rho_0 E\left(\boldsymbol{\eta}\right) = {} & C_{11}P_1 + C_{12}P_2 + C_{13}P_3 + C_{33}P_4 + C_{44}P_5 + C_{111}P_6 + C_{222}P_7 + C_{333}P_8 + \\ & C_{133}P_9 + C_{113}P_{10} + C_{112}P_{11} + C_{123}P_{12} + C_{144}P_{13} + C_{155}P_{14} + C_{344}P_{15}\end{aligned} \tag{A17}$$

$$P_1 = \frac{\eta_1^2}{2} + \frac{\eta_2^2}{2} + \frac{\eta_6^2}{4}, \tag{A18a}$$

$$P_2 = -\frac{\eta_6^2}{4} + \eta_1\eta_2, \tag{A18b}$$

$$P_3 = \eta_1\xi + \eta_2\xi, \tag{A18c}$$

$$P_4 = \frac{\xi^2}{2}, \tag{A18d}$$

$$P_5 = \frac{\eta_4^2}{2} + \frac{\eta_5^2}{2}, \tag{A18e}$$

$$P_6 = \frac{\eta_1^3}{6} + \frac{\eta_1\eta_2^2}{2} - \frac{\eta_1\eta_6^2}{4} + \frac{\eta_2\eta_6^2}{4}, \tag{A18f}$$

$$P_7 = \frac{\eta_2^3}{6} - \frac{\eta_1\eta_2^2}{2} - \frac{\eta_2\eta_6^2}{8} + 3\frac{\eta_1\eta_6^2}{8}, \tag{A18g}$$

$$P_8 = \frac{\xi^3}{6}, \tag{A18h}$$

$$P_9 = \frac{\eta_1\xi^2}{2} + \frac{\eta_2\xi^2}{2}, \tag{A18i}$$

$$P_{10} = \frac{\xi\eta_1^2}{2} + \frac{\xi\eta_2^2}{2} + \frac{\xi\eta_6^2}{4}, \tag{A18j}$$

$$P_{11} = \frac{\eta_1^2\eta_2}{2} + \frac{\eta_1\eta_2^2}{2} - \frac{\eta_6^2\eta_1}{8} - \frac{\eta_6^2\eta_2}{8}, \tag{A18k}$$

$$P_{12} = \eta_1\eta_2\xi - \frac{\xi\eta_6^2}{4}, \tag{A18l}$$

$$P_{13} = \frac{\eta_1\eta_4^2}{2} + \frac{\eta_2\eta_5^2}{2} - \frac{\eta_4\eta_5\eta_6}{2}, \tag{A18m}$$

$$P_{14} = \frac{\eta_2\eta_4^2}{2} + \frac{\eta_1\eta_5^2}{2} + \frac{\eta_4\eta_5\eta_6}{2}, \tag{A18n}$$

$$P_{15} = \frac{\xi\eta_4^2}{2} + \frac{\xi\eta_5^2}{2} \tag{A18o}$$

Similar to the cubic materials, we now invoke the symmetry of the material and the specifics of the loading condition to simplify the resulting expressions that relate stress, strain and elastic constants. As a hexagonal material is loaded uniaxially along c by a strain ξ, it contracts or expands in the basal plane by an amount $\eta_1 = \eta_2 = \bar{\eta}$. In addition, no shear strain can result from this type of loading, hence $\eta_4 = \eta_5 = \eta_6 = 0$. These constraints simplify Eq. A17 considerably, to the expression shown in Eq. A19.

$$\rho_0 E(\boldsymbol{\eta}) = \left(\frac{2C_{111}}{3} + C_{112} - \frac{C_{222}}{3}\right)\bar{\eta}^3 + (C_{11} + C_{12} + C_{113}\xi + C_{123}\xi)\,\bar{\eta}^2 + \left(C_{113}\xi^2 + 2C_{23}\xi\right)\bar{\eta} + \frac{C_{333}}{6}\xi^3 + \frac{C_{33}}{2}\xi^2 \tag{A19}$$

The equilibrium strain in the basal plane due to the application of ξ is obtained by a strain-energy minimization of Eq. A19 with respect to $\bar{\eta}$. This equation and the resulting solution of the type $\bar{\eta} = \bar{\eta}(\xi)$ are rather long and are not shown here.

Similar to the case of a cubic crystal, the component S_{33} of the second Piola-Kirchhoff stress tensor can be obtained from Eq. A7 and is shown in Eq. A20. All other components in $\mathbf{S}$ are zero and the same is true for σ.

$$S_{33} = 2C_{23}\bar{\eta} + C_{33}\xi + (C_{113} + C_{123})\,\bar{\eta}^2 + \frac{C_{333}}{2}\xi^2 + 2C_{133}\bar{\eta}\xi \tag{A20}$$

The Cauchy (true) stress component σ_{33} can now be calculated for every strain ξ from Eq. A9. The detailed procedure is summarized below.

1. Consider an applied strain ξ
2. Compute the resulting strain (Poisson contraction) $\bar{\eta}$ from Eq. A19
3. Compute S_{33} from Eq. A20
4. Compute σ_{33} from Eq. A9

Appendix B: Derivation of Wallace tensors

The Wallace tensor is defined in Eq. B1, where the terms C'_{ijkl} represent the elastic constants in the deformed configuration and σ_{ij} are the components of the Cauchy (true) stress tensor. Further, δ is the Kronecker delta function. The eigenvalues of the symmetrized Wallace tensor govern the mechanical stability of a solid under stress and its eigenvectors describe the type of deformation (e.g. shear or tensile deformation modes).

For the loading situations considered in this work, the Cauchy stress tensor can be written out as in Eq. B1. Note that σ_{33} can be expressed as a function of only the SOEC's, TOEC's and ξ (see Eq. B2). Similarly, C'_{ijkl} can be expressed in terms of the SOEC's, TOEC's and ξ (see Eq. B2). Hence, the formalism proposed in this work can be used to express the mechanical stability of any solid under uniaxial loading in terms of material constants and the applied strain.

$$B_{ijkl} = C'_{ijkl} + \frac{1}{2}\left(\sigma_{il}\delta_{jk} + \sigma_{jl}\delta_{ik} + \sigma_{ik}\delta_{jl} + \sigma_{jk}\delta_{il} - 2\sigma_{ij}\delta_{kl}\right) \tag{B1}$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}\left(C_{ijkl}, C_{ijklmn}, \xi\right) \tag{B2}$$

$$C'_{ijkl} = C'_{ijkl}\left(C_{ijkl}, C_{ijklmn}, \xi\right) \tag{B3}$$

$$\boldsymbol{\sigma} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix} \tag{B4}$$

$$\bar{B}_{ij} = \frac{1}{2}\left(B_{ij} + B_{ji}\right) \tag{B5}$$

Note that the Wallace tensor as defined in Eq. B1 does not in general lead to a symmetric tensor. The stability is in fact governed by the symmetrized Wallace tensor, denoted by $\bar{B}$, and defined in Eq. B2 (in Voigt notation). The simplicity of Eq. B4 allows Eq. B1 to be written in a particularly simple form. Expressions are derived specifically for cubic and hexagonal materials. Note that the term $\frac{1}{2}\left(\sigma_{il}\delta_{jk} + \sigma_{jl}\delta_{ik} + \sigma_{ik}\delta_{jl} + \sigma_{jk}\delta_{il} - 2\sigma_{ij}\delta_{kl}\right)$ in the Wallace tensor will be identical for cubic and hexagonal materials considered in this work, and the difference comes in only in the symmetry of C'_{ijkl}. In Voigt notation, the term $\frac{1}{2}\left(\sigma_{il}\delta_{jk} + \sigma_{jl}\delta_{ik} + \sigma_{ik}\delta_{jl} + \sigma_{jk}\delta_{il} - 2\sigma_{ij}\delta_{kl}\right)$ is shown in Eq. B6.

$$\frac{1}{2}\left(\sigma_{il}\delta_{jk}+\sigma_{jl}\delta_{ik}+\sigma_{ik}\delta_{jl}+\sigma_{jk}\delta_{il}-2\sigma_{ij}\delta_{kl}\right)=\begin{bmatrix}0&0&0&0&0&0\\0&0&0&0&0&0\\-\sigma_{33}&-\sigma_{33}&\sigma_{33}&0&0&0\\0&0&0&\frac{\sigma_{33}}{2}&0&0\\0&0&0&0&\frac{\sigma_{33}}{2}&0\\0&0&0&0&0&0\end{bmatrix} \tag{B6}$$

1. Cubic crystal system

For cubic materials, 3 independent SOEC's exist, which are taken here to be C_{11}, C_{12} and C_{44}. Further, 6 independent TOEC's exist, chosen here as C_{111}, C_{112}, C_{123}, C_{144}, C_{155} and C_{456}. Employing Eq. 1 and subsequently symmetrizing according to Eq. B5 yields the symmetrized Wallace tensor (in Voigt notation) as shown in B7.

$$\bar{B}_{ij}=\begin{bmatrix}C'_{11}&C'_{12}&C'_{13}-\frac{\sigma_{33}}{2}&0&0&0\\C'_{12}&C'_{11}&C'_{13}-\frac{\sigma_{33}}{2}&0&0&0\\C'_{13}-\frac{\sigma_{33}}{2}&C'_{13}-\frac{\sigma_{33}}{2}&C'_{33}+\sigma_{33}&0&0&0\\0&0&0&C'_{44}+\frac{\sigma_{33}}{2}&0&0\\0&0&0&0&C'_{44}+\frac{\sigma_{33}}{2}&0\\0&0&0&0&0&C'_{66}\end{bmatrix} \tag{B7}$$

2. Hexagonal crystal system

Similar to cubic materials, the Wallace tensor for hexagonal materials can be expressed in terms of the Cauchy stress component σ_{33} and the deformed elastic constants, both of which can be derived from the SOEC's, TOEC's and the applied strain ξ along the c-axis. For this crystal system, we have 5 independent SOEC's, taken to be C_{11}, C_{12}, C_{13}, C_{33} and C_{44}. Employing Eq. 1 and subsequently symmetrizing according to Eq. B5 yields the symmetrized Wallace tensor (in Voigt notation) as shown in B8.

$$\bar{B}_{ij}=\begin{bmatrix}C'_{11}&C'_{12}&C'_{13}-\frac{\sigma_{33}}{2}&0&0&0\\C'_{12}&C'_{11}&C'_{13}-\frac{\sigma_{33}}{2}&0&0&0\\C'_{13}-\frac{\sigma_{33}}{2}&C'_{13}-\frac{\sigma_{33}}{2}&C'_{33}+\sigma_{33}&0&0&0\\0&0&0&C'_{44}+\frac{\sigma_{33}}{2}&0&0\\0&0&0&0&C'_{44}+\frac{\sigma_{33}}{2}&0\\0&0&0&0&0&\frac{C'_{11}-C'_{12}}{2}\end{bmatrix} \tag{B8}$$

Appendix C: Derivation of deformed elastic constants

In this section, derivations are presented for the deformed elastic constants and their dependence on the undeformed elastic constants, the TOEC's and the strain state experienced by the material.

1. General considerations

A priori, we know that the tensor representing the TOEC's can have $6^3 = 216$ possible unique elements. This number, however, does not reflect Voigt symmetry. We start by noting that the completely diagonal elements, C_{iiiiii}, for example, have only one possibility. Hence, this gives 6 unique elements. The next type of entry has two identical indices, and 1 different index. There are six ways to choose the repeated index, and 5 ways to choose the lone index. This implies that are 30 unique elements here as well. Each of these elements, however, corresponds to 3 of the elements C_{mnp} for a total of 90 elements of the general Voigt tensor.

The remaining elements all have unique n, m, p. There are 6 ways to choose the first element, 5 ways to choose the second, and 4 ways to choose the third, for a

total of 120 ways to choose these. However, the choices are repeated, so that there are only 20 possibilities. Each of these 20 possibilities, however, can be represented six times for a total of 120 elements in the form C_{nmp}.

Adding all these elements together yields $6 + 90 + 120 = 216$, so we appear to have found them all. The net result is that there are potentially 56 unique elements of the third order elastic constants tensor. We can use this to simplify the rules that come out of the generic analysis.

We propose the following structure for defining the unique 56 elements that might appear in our tensor. The Voigt diagonal elements will be given by the only possibility. The tensor elements that have a repeated index will have that repeated index appear in the first two entries. The tensor elements that have three unique indices will always be sorted so that the indices are in increasing order.

In relating tensor components to each other, the following transformation relations are used extensively. For generic second order tensors L_{ij} (e.g. stress tensors, thermal conductivity tensors), it is well-known that they transform according to:

$$L_{ij} = T_{ik}T_{jl}L_{kl} \tag{C1}$$

By enumerating all possible transformations under the elements of a crystallographic group, it is then possible to obtain restrictions on the components of the tensor, e.g. relations among components or certain components being identically equal to zero. This is the basis of Neumann's principle. Similar transformation rules apply to tensors of order 4 (e.g. SOEC's) and order 6 (e.g. TOEC's):

$$C_{ijkl} = T_{im}T_{jn}T_{ko}T_{lp}C_{mnop} \tag{C2}$$

$$C_{ijklrs} = T_{im}T_{jn}T_{ko}T_{lp}T_{rq}T_{st}C_{mnopqt} \tag{C3}$$

The deformed elastic constants can be obtained by considering a large deformation strain characterized by the tensor $\boldsymbol{\eta}^0$, with a small symmetric deformation strain tensor $\boldsymbol{\beta}$ applied on top of that. A point in the solid with no applied strain is defined as $\boldsymbol{X}$. $\boldsymbol{X}$ is mapped to a point ($\boldsymbol{x^0}$) under a finite strain of $\boldsymbol{\eta}^0$ by the deformation gradient $F^0_{jm} = \frac{\partial x^0_j}{\partial X_m}$. In addition, $\boldsymbol{X}$ is mapped to a point ($\boldsymbol{x}$) in the combined finite and infinitesimal strain state, denoted as $\boldsymbol{\eta}$, by the deformation gradient $F_{jm} = \frac{\partial x_j}{\partial X_m}$. Because $\boldsymbol{\beta}$ is an infinitesimal strain,

$$x_j = x^0_j + \beta_{jm}x^0_m. \tag{C4}$$

With these three strain states defined the deformed elastic constants can be defined as,

$$C'_{klmn} = \rho(\boldsymbol{\eta}^0)\left(\frac{\partial^2 E}{\partial\beta_{kl}\partial\beta_{mn}}\right)_{\boldsymbol{\beta'},\boldsymbol{\eta}^0}. \tag{C5}$$

By substituting equation A4 into equation C5, the deformed elastic constants can be derived purely in terms of the SOEC's, TOEC's, and $\boldsymbol{\eta}^0$, provided that the deformation gradients can be written in terms of the applied finite strain (see equations A5 and A6).

2. Cubic crystal system

Below is a list of the generators used in the cubic calculations. They correspond to a four-fold rotation along the [001] axis, a mirror plane operating on (010), and a three-fold rotation along [111].

$$\boldsymbol{R}_{4[001]} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{C6}$$

$$\boldsymbol{R}_{m(010)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{C7}$$

$$\boldsymbol{R}_{3[111]} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \tag{C8}$$

The size of the resulting group is 48, and each of these elements corresponds to a transformation matrix. We now use the tensor transformation rules and consider all possible transformations, imposed by the symmetry-group operations. We use the equations for the tensor transformations and consider all possible transformations, imposed by the symmetry-group operations.

Writing out the transformation equations for the tensor of order 6, C_{ijklrs}, and using all 48 elements of the group we obtain a grand total of $48 \cdot 3^6 = 34,992$ equations relating the components of this tensor. Many of these equations are however not independent. Mathematica is used to find the independent constraint equations, of which there are 50 in total. This implies that there are 56-50 = 6 independent TOEC's. Here, the following 6 independent TOEC's are chosen (note that this choice is not unique) in Voigt notation: C_{111}, C_{112}, C_{123}, C_{144}, C_{166}, C_{456}.

The deformed elastic constants are finally obtained using Eq. C5 and are given as follows:

$$C'_{11} = C_{11} + \eta(3C_{11} + C_{111} + C_{112} + C_{12}) + \xi(-C_{11} + C_{112} + C_{12}), \tag{C9a}$$
$$C'_{12} = C_{12} + 2\eta(C_{112} + C_{12}) + \xi(C_{123} - C_{12}), \tag{C9b}$$
$$C'_{13} = C_{12} + \eta(C_{112} + C_{123}) + \xi(C_{112} + C_{12}), \tag{C9c}$$
$$C'_{33} = C_{11} + 2\eta(-C_{11} + C_{112} + 2C_{12}) + \xi(4C_{11} + C_{111}), \tag{C9d}$$
$$C'_{44} = C_{44} + \eta\left(\frac{1}{4}C_{11} + \frac{3}{4}C_{12} + C_{144} + C_{166}\right) + \xi\left(\frac{1}{4}C_{11} + \frac{1}{4}C_{12} + C_{166} + C_{44}\right), \tag{C9e}$$
$$C'_{66} = C_{66} + \eta\left(2C_{166} + \frac{1}{2}C_{11} + \frac{1}{2}C_{12} + 2C_{66}\right) + \xi\left(-C_{66} + \frac{1}{2}C_{12} + C_{144}\right) \tag{C9f}$$

3. Hexagonal crystal system

For the HCP system, the space group is $P6_3/mmc$ with a point group of $6/mmm$. We choose the following 3 generators and multiply them all together to form a group.

$$R_1 = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{C10}$$

$$R_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{C11}$$

$$R_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{C12}$$

It can easily be established that the length of the resulting group is 24, as it should be. Each of these elements corresponds to a transformation matrix. We now use the tensor transformation rules and consider all possible transformations, imposed by the symmetry-group operations.

Writing out the transformation equations for the tensor of order 6, C_{ijklrs}, and using all 24 elements of the group we obtain a grand total of $24 \cdot 3^6 = 17,496$ equations relating the components of this tensor. Many of these equations are however not independent. Mathematica is used to find the independent constraint equations, of which there are 46 in total. This implies that there are 56-46 = 10 independent TOEC's. Here, the following 10 independent TOEC's are chosen (note that this choice is not unique) in Voigt notation: C_{663}, C_{662}, C_{661}, C_{553}, C_{552}, C_{551}, C_{333}, C_{332}, C_{222}, C_{223}. In addition, the following set of relations is found that can be used to convert between the various choices of independent TOEC's:

$$
\begin{aligned}
C_{111} &= C_{222} - C_{661} + C_{662} \\
C_{133} &= C_{332} \\
C_{113} &= C_{223} \\
C_{112} &= C_{222} - 2C_{661} - 2C_{662} \\
C_{123} &= C_{222} - 2C_{663} \\
C_{144} &= C_{552} \\
C_{155} &= C_{551} \\
C_{344} &= C_{553} \\
C_{654} &= \frac{1}{2}\left(C_{551} - C_{552}\right) \\
C_{344} &= C_{553}
\end{aligned}
\tag{C13}
$$

The deformed elastic constants are finally obtained using Eq. C5 and are given as follows:

$$C'_{11} = C_{11} + \eta(3C_{11} + C_{12} + C_{111} + C_{112}) + \xi(-C_{11} + C_{113} + C_{13}), \tag{C14a}$$

$$C'_{12} = C_{12} + \eta(2C_{12} + \frac{5}{3}C_{112} + \frac{1}{3}C_{111} - \frac{4}{3}C_{166}) + \xi(-C_{12} + C_{123}), \tag{C14b}$$

$$C'_{13} = C_{13} + \eta(C_{123} + C_{113}) + \xi(C_{13} + C_{133}), \tag{C14c}$$

$$C'_{33} = C_{33} + \eta(2C_{13} - 2C_{33} + 2C_{133}) + \xi(4C_{33} + C_{333}), \tag{C14d}$$

$$C'_{44} = C_{44} + \eta\left(\frac{1}{4}C_{11} + \frac{1}{4}C_{12} + \frac{1}{2}C_{13} + C_{144} + C_{155}\right) + \xi\left(C_{44} + C_{355} + \frac{1}{4}C_{33} + \frac{1}{4}C_{13}\right), \tag{C14e}$$

$$C'_{66} = \frac{1}{2}\left(C'_{11} - C'_{12}\right) \tag{C14f}$$

Appendix D: Details of calculating TOEC's

1. General method

Below is an outline of the method used to calculate the third-order elastic constants.

The third-order elastic constants are defined as

$$C_{ijklmn} = \rho_0 \frac{\partial^3 E}{\partial\eta_{ij}\partial\eta_{kl}\partial\eta_{mn}}|_{\boldsymbol{\eta}=0}. \tag{D1}$$

If the TOEC contains Voigt symmetry, but no point symmetry other than the identity, the sixth-order elastic tensor will consist of 56 unique constants. By evaluating the second derivative of the stress components with respect to η for 21 unique strain states defined in Eqs. D2.

$$\boldsymbol{\eta}^1 = \begin{pmatrix} \eta & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{D2a}$$
$$\boldsymbol{\eta}^2 = \begin{pmatrix} 0 & \eta & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{D2b}$$
$$\boldsymbol{\eta}^3 = \begin{pmatrix} 0 & 0 & \eta & 0 & 0 & 0 \end{pmatrix}, \tag{D2c}$$
$$\boldsymbol{\eta}^4 = \begin{pmatrix} 0 & 0 & 0 & 2\eta & 0 & 0 \end{pmatrix}, \tag{D2d}$$
$$\boldsymbol{\eta}^5 = \begin{pmatrix} 0 & 0 & 0 & 0 & 2\eta & 0 \end{pmatrix}, \tag{D2e}$$
$$\boldsymbol{\eta}^6 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 2\eta \end{pmatrix}, \tag{D2f}$$
$$\boldsymbol{\eta}^7 = \begin{pmatrix} \eta & \eta & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{D2g}$$
$$\boldsymbol{\eta}^9 = \begin{pmatrix} \eta & 0 & \eta & 0 & 0 & 0 \end{pmatrix}, \tag{D2h}$$
$$\boldsymbol{\eta}^{10} = \begin{pmatrix} \eta & 0 & 0 & 2\eta & 0 & 0 \end{pmatrix}, \tag{D2i}$$
$$\boldsymbol{\eta}^{11} = \begin{pmatrix} \eta & 0 & 0 & 0 & 2\eta & 0 \end{pmatrix}, \tag{D2j}$$
$$\boldsymbol{\eta}^{12} = \begin{pmatrix} \eta & 0 & 0 & 0 & 0 & 2\eta \end{pmatrix}, \tag{D2k}$$
$$\boldsymbol{\eta}^{13} = \begin{pmatrix} 0 & \eta & 0 & 2\eta & 0 & 0 \end{pmatrix}, \tag{D2l}$$
$$\boldsymbol{\eta}^{14} = \begin{pmatrix} 0 & \eta & 0 & 0 & 2\eta & 0 \end{pmatrix}, \tag{D2m}$$
$$\boldsymbol{\eta}^{15} = \begin{pmatrix} 0 & \eta & 0 & 0 & 0 & 2\eta \end{pmatrix}, \tag{D2n}$$
$$\boldsymbol{\eta}^{16} = \begin{pmatrix} 0 & 0 & \eta & 2\eta & 0 & 0 \end{pmatrix}, \tag{D2o}$$
$$\boldsymbol{\eta}^{17} = \begin{pmatrix} 0 & 0 & \eta & 0 & 2\eta & 0 \end{pmatrix}, \tag{D2p}$$
$$\boldsymbol{\eta}^{18} = \begin{pmatrix} 0 & 0 & \eta & 0 & 0 & 2\eta \end{pmatrix}, \tag{D2q}$$
$$\boldsymbol{\eta}^{19} = \begin{pmatrix} 0 & 0 & 0 & 2\eta & 2\eta & 0 \end{pmatrix}, \tag{D2r}$$
$$\boldsymbol{\eta}^{20} = \begin{pmatrix} 0 & 0 & 0 & 2\eta & 0 & 2\eta \end{pmatrix}, \tag{D2s}$$
$$\boldsymbol{\eta}^{21} = \begin{pmatrix} 0 & 0 & 0 & 0 & 2\eta & 2\eta \end{pmatrix}, \tag{D2t}$$
$$\tag{D2u}$$

results in a vector, $\boldsymbol{\tau}$, containing 126 terms that consist of the 56 TOEC. Writing the TOEC as a 56×1 array, $\boldsymbol{\xi}$, the 126×56 matrix, $\boldsymbol{A}$, can be defined as

$$A_{ik} = \frac{\partial \tau_i}{\partial \xi_k}. \tag{D3}$$

Defining $\boldsymbol{B}$ to be the pseudoinverse of $\boldsymbol{A}$ the TOEC can be written as

$$\xi_i = B_{ik}\tau_k. \tag{D4}$$

The components of $\boldsymbol{\tau}$ were evaluated numerically using the finite difference method. A 9 point central difference stencil about $\eta = 0$ was used to calculate the second derivative of the 2nd Piola-Kirchhoff stress components. While the maximum strain used in the finite difference calculations is system dependent and determined from convergence testing with respect to the TOEC, a maximum strain of $\eta_{max} = 0.05$ has been shown to be appropriate for most systems studied.

In the calculation of the TOEC no considerations with regards to symmetry are given. In the case where the point group of the crystal is larger than the identity or it is desired to approximate the closest tensor of a higher symmetry (such as in the case of a solid solution), the TOEC must be symmetrized as follows

$$\hat{C}_{ijklmn} = \frac{1}{n_G} \sum_{\alpha=1}^{n_G} a_{ip}^{(\alpha)} a_{jq}^{(\alpha)} a_{kr}^{(\alpha)} a_{ls}^{(\alpha)} a_{mt}^{(\alpha)} a_{nv}^{(\alpha)} C_{pqrstu}, \tag{D5}$$

where n_G is the number of elements in the group, and $a_{ip}^{(\alpha)}$, the transformation matrix associated with the α^{th} element of the group. Note that Einstein summation is applied to all Latin subscripts.

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[1] T. Li, J. Morris Jr, N. Nagasako, S. Kuramoto, and D. Chrzan, Physical review letters **98**, 105503 (2007).
[2] D. Clatterbuck, D. Chrzan, and J. Morris, Acta Materialia **51**, 2271 (2003).
[3] A. Kelly and N. H. Macmillan, Oxford University Press, Walton Street, Oxford OX 2 6 DP, UK, 1986. (1986).
[4] H. Wang and M. Li, Physical Review Letters **111**, 065507 (2013).
[5] D. M. Clatterbuck, C. R. Krenn, M. L. Cohen, and J. W. Morris, Phys. Rev. Lett. **91**, 135501 (2003).
[6] L. Qi and D. Chrzan, Phys. Rev. Lett. **112**, 115503 (2014).
[7] N. Macmillan, in Atomistics of fracture (Springer, 1983) pp. 95–165.
[8] D. Roundy, C. Krenn, M. L. Cohen, and J. Morris Jr, Philosophical magazine A **81**, 1725 (2001).
[9] H. Wang and M. Li, Journal of Physics: Condensed Matter **21**, 455401 (2009).
[10] D. Roundy, C. R. Krenn, M. L. Cohen, and J. W. Morris, Phys. Rev. Lett. **82**, 2713 (1999).
[11] X. Li, S. Schönecker, J. Zhao, B. Johansson, and L. Vitos, Phys. Rev. B **87**, 214203 (2013).
[12] M. Šob, L. Wang, and V. Vitek, Materials Science and Engineering: A **234**, 1075 (1997).
[13] F. Milstein and S. Chantasiriwan, Phys. Rev. B **58**, 6006 (1998).
[14] J. Pokluda, M. Černỳ, P. Šandera, and M. Šob, Journal of computer-aided materials design **11**, 1 (2004).
[15] H. Wang and M. Li, Journal of Physics: Condensed Matter **22**, 295405 (2010).
[16] J. Morris Jr and C. Krenn, Philosophical Magazine A **80**, 2827 (2000).
[17] J. Wang, S. Yip, S. Phillpot, and D. Wolf, Physical Review Letters **71**, 4182 (1993).
[18] M. de Jong, S. van der Zwaag, and M. Sluiter, International Journal of Materials Research **103**, 972 (2012).
[19] M. de Jong, L. Qi, D. L. Olmsted, A. van de Walle, and M. Asta, Physical Review B **93**, 094101 (2016).
[20] H. Wang and M. Li, Journal of Physics: Condensed Matter **24**, 245402 (2012).
[21] D. C. Wallace, Thermodynamics of crystals (Courier Corporation, 1998).
[22] J. R. Ray, Computer physics reports **8**, 109 (1988).
[23] J. Wang, J. Li, S. Yip, S. Phillpot, and D. Wolf, Physical Review B **52**, 12627 (1995).

[24] H. Wang and M. Li, Physical Review B **85**, 104103 (2012).
[25] M. Łopuszyński and J. A. Majewski, Physical Review B **76**, 045202 (2007).
[26] M. Lopuszynski and J. Majewski, Acta Physica Polonica-Series A General Physics **112**, 443 (2007).
[27] M. de Jong, W. Chen, T. Angsten, A. Jain, R. Notestine, A. Gamst, M. Sluiter, C. K. Ande, S. van der Zwaag, J. J. Plata, et al., Scientific Data **2** (2015).
[28] M. De Jong, W. Chen, H. Geerlings, M. Asta, and K. A. Persson, Scientific data **2** (2015).
[29] C. M. Kube and M. de Jong, Journal of Applied Physics **120**, 165105 (2016).
[30] M. de Jong, W. Chen, R. Notestine, K. Persson, G. Ceder, A. Jain, M. Asta, and A. Gamst, Scientific Reports **6** (2016).
[31] A. Van de Walle, P. Tiwary, M. De Jong, D. Olmsted, M. Asta, A. Dick, D. Shin, Y. Wang, L.-Q. Chen, and Z.-K. Liu, Calphad **42**, 13 (2013).
[32] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996).
[33] G. Kresse and J. Hafner, Phys. Rev. B **47**, 558 (1993).
[34] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).
[35] P. E. Blöchl, Phys. Rev. B **50**, 17953 (1994).
[36] G. Kresse and D. Joubert, Phys. Rev. B **59**, 1758 (1999).
[37] M. Methfessel and A. T. Paxton, Phys. Rev. B **40**, 3616 (1989).
[38] H. J. Monkhorst and J. D. Pack, Phys. Rev. B **13**, 5188 (1976).
[39] C. Krenn, D. Roundy, M. L. Cohen, D. Chrzan, and J. Morris Jr, Physical Review B **65**, 134111 (2002).
[40] F. Schmidt and H. R. Ogden, The engineering properties of tantalum and tantalum alloys, Tech. Rep. (DTIC Document, 1963).
[41] H. McCoy Jr, R. L. Stephenson, and J. Weir Jr, Mechanical Properties of Some Refractory Metals and Their Alloys, Tech. Rep. (Oak Ridge National Lab., Tenn., 1964).
[42] F. F. Schmidt and H. R. Ogden, The engineering properties of tungsten and tungsten alloys, Tech. Rep. (DTIC Document, 1963).
[43] P. G. Adams and C. L. Dotson, Mechanical and physical properties of TZM molybdenum alloy sheet and of tungsten sheet, Tech. Rep. (DTIC Document, 1965).
[44] A. Wronski, A. Chilton, and E. Capron, Acta Metallurgica **17**, 751 (1969).
[45] P. Gumbsch, J. Riedle, A. Hartmaier, and H. F. Fischmeister, Science **282**, 1293 (1998).
[46] H. Smith, J. Hum, A. Donlevy, and C. d. Hunt, Journal of the Less Common Metals **2**, 69 (1960).
[47] A. Knapton, Journal of the Less Common Metals **2**, 113 (1960).
[48] W. D. Klopp, Journal of the Less Common Metals **42**, 261 (1975).
[49] C. Krenn, D. Roundy, J. Morris, and M. L. Cohen, Materials Science and Engineering: A **319**, 111 (2001).
[50] W. Luo, D. Roundy, M. L. Cohen, and J. Morris Jr, Physical Review B **66**, 094110 (2002).
[51] Y.-L. Liu, H.-B. Zhou, Y. Zhang, S. Jin, and G.-H. Lu, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms **267**, 3282 (2009).
[52] M. de Jong, D. L. Olmsted, A. van de Walle, and M. Asta, Physical Review B **86**, 224101 (2012).
[53] M. de Jong, J. Kacher, M. Sluiter, L. Qi, D. Olmsted, A. Van de Walle, J. Morris Jr, A. Minor, and M. Asta, Physical review letters **115**, 065501 (2015).
[54] E. M. Savitskii, Physical metallurgy of refractory metals and alloys (Springer Science & Business Media, 2012).
[55] D. Webster, Beryllium Science and Technology, Vol. 2 (Plenum Publishing Corporation, 1979).
[56] M. I. El Guindy, Precious Metals 1982: Proceedings of the Sixth International Precious Metals Institute Conference, Held in Newport Beach, California, June 7-11, 1982 (Elsevier, 2013).
[57] R. Nunes, ASM Handbook: Properties and Selection: Nonferrous Alloys and Special-purpose Materials, Vol. 2 (ASM International, 1992).
[58] S. Pugh, The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science **45**, 823 (1954).