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Melting anisotropy in crystalline solids

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Abstract

Despite the long and extensive history of melting studies, experiments to determine the dependence of melting on crystal orientation are lacking. Using longitudinal sound speed measurements in aluminum single crystals shock compressed along $\langle 100 \rangle$ and $\langle 110 \rangle$ to 168 GPa, we address this need and show that the melting transition (both onset and completion) is strongly anisotropic. The present findings demonstrate the need to consider the role of deformation induced lattice defects on the melting transition and provide a general approach to examine melting anisotropy in crystalline solids.

Melting of crystalline solids is likely the structural transition that everyone is most familiar with. Melting studies at ambient pressure and high pressures provide the temperature (T) and pressure (P) phase diagrams that are important for understanding states of matter in nearly all scientific disciplines and utilized in a vast range of materials technologies. The literature regarding the melting transition and related scientific studies is enormous and we provide a representative list of publications spanning different disciplines [1–18]. Despite the long history and vast scientific literature regarding the melting transition, a fundamental and intriguing scientific question has not been experimentally addressed to date: does the melting of a crystalline solid depend on its orientation? Stated differently, is melting an anisotropic phenomenon? Although differing theoretical suggestions have been put forward over the years [19–23], experimental measurements to address this question are lacking.

Plane shock wave experiments provide an ideal approach to examine the issue of melting anisotropy because shock waves – resulting in a near-discontinuous change in temperature and pressure – can be propagated precisely along different crystal orientations. While there is a long history of using shock wave compression for studying melting at high pressures [24–33], shock experiments have not been utilized to date to examine the dependence of melting on crystal orientation. Some recent papers have reported on shock-induced melting in single crystals [34–36], but none of these studies examined the issue of melting anisotropy.

We report here on the use of longitudinal sound speed measurements in the shock compressed state – a well-established method to study shock-induced melting [25–27,29,32,33,35] – to examine the melting transition in Al single crystals shock compressed along $\langle 100 \rangle$ and $\langle 110 \rangle$ orientations. Our results demonstrate conclusively the significant anisotropy associated with the

melting of Al single crystals. Mechanistic issues to understand this novel finding are discussed in this work.

Al single crystals were chosen for this first study because of the following factors: single crystal Al is a soft, face-centered-cubic (fcc) metal with a low anisotropy factor ($\frac{2C_{44}}{C_{11}-C_{12}} = 1.21$) [37] – value of these elastic constants C_{11} , C_{12} , and C_{44} are listed in supplementary material (SM) [38] (see also references [39–50] therein); polycrystalline Al has been studied in shock compression to high stresses [51–55] and theoretical efforts regarding the development of Al equations of state (EOS) have been well documented [54,56–63]; accurate pressure (P) – volume (V) states under shock compression (referred to as Hugoniot data) and longitudinal sound speeds in shocked states have been obtained to ~70 GPa for three different crystal orientations for solid phase Al [37]; and <100> LiF optical windows [35] used for laser-interferometry measurements in our experiments are a near-ideal impedance match to Al crystals, resulting in high precision data.

We note that the solid phase results under shock compression (to ~70 GPa) in Ref. 37 showed two interesting features that are relevant to the present work: the P – V states for the three orientations were nearly identical, demonstrating negligible anisotropy; in contrast, the longitudinal sound speeds demonstrated significant anisotropy and were not converging even for 50 percent compression (and the corresponding temperature rise). The <100> and <110> orientations showed the largest differences, and, thus, were selected for the present work. Before the present work, we did not know if the differences observed in the solid state at lower stresses and temperatures would continue at higher stresses and temperatures – and through the melt transition.

Using the plate impact experimental configuration shown in Fig. 1, $\langle 100 \rangle$ and $\langle 110 \rangle$ Al single crystals were shock compressed to peak stresses ranging between 70 and 168 GPa. Experimental details regarding the fifteen experiments conducted in this study are provided in the supplementary material (SM) [38], and only a brief summary is presented here. The targets consisted of an Al single crystal front buffer bonded to an Al single crystal sample of the same orientation backed by a LiF (100) optical window. The sample assembly was impacted using copper (Cu) impactors, launched using a 2-stage gas gun. Wave profile measurements were obtained using laser interferometry at the Al sample/LiF window interface (green arrow-VISAR [64] and red arrow-PDV [65]) and at the back of the buffer (red arrows-PDV [65]). In all experiments, a single jump followed by a constant peak state was observed before the arrival of the release wave from the back of the impactor (Fig. S2 (SM) [38]). The measured release wave profiles were smooth, typical of the unloading response for crystalline solids shock compressed to high pressures [35,66].

From shock wave arrival times at the back of the buffer and at the sample/window interface, shock velocities were determined with high precision. Because the LiF (100) window is an excellent impedance match to the Al samples, wave reflections from the sample/window interface are negligible – resulting in accurate measurements of the release onset velocities. The experimental parameters relevant to these fifteen experiments are summarized in Table S2 in SM [38]. The methods used to analyze the wave profiles are well established and are presented in Section S3 in SM [38]; only the results are presented and discussed here. The in-material stresses, densities, and the longitudinal sound speeds (and moduli) in the shocked state are listed in Table S3 in SM [38].

Following the analysis described in Section S3 in SM [38], the shock wave velocity (U_s)–particle velocity (u_p) results – and the corresponding stress-volume states – are plotted along with previously published lower stress results [37] in Fig. 2. The black solid line denotes the linear relation (Fig. 2(a)) obtained from a weighted fit to all data ranging from 43 to 168 GPa. The shock response for Al single crystals is well described in Fig. 2(a) using the following equation: $U_s = C_0 + Su_p$, km/s where $C_0 = 5.361$ km/s, and $S = 1.316$. We note that Figs. 2(a) and 2(b) constitute completely equivalent representations of the shock compressed states. Within experimental uncertainty, the $U_s - u_p$ results in Fig. 2 show that the peak states of Al shocked along $\langle 100 \rangle$ and $\langle 110 \rangle$ orientations are nearly identical to ~ 168 GPa, with no discernable anisotropy. For completeness, these data were individually fitted for each orientation and are presented in SM [38]; differences between the two fits are negligible.

The longitudinal sound speeds, listed in Table S3 [38], are plotted vs. longitudinal stress and density compression in Fig. 3; lower stress results from Ref. 37 are also shown in the figure. For visual clarity, the results for the $\langle 100 \rangle$ and $\langle 110 \rangle$ orientations are separated into Fig. 3(a) and Fig. 3(b), respectively. The results from Fig. 3 were used to determine the longitudinal elastic moduli in the shocked state, and the same are plotted as a function of longitudinal stress and density compression in Fig. 4. Similar to Fig. 3, the results for the two orientations are shown separately in Fig. 4(a) and Fig. 4(b). We note that the density compression corresponding to the peak stresses are shown along the top axis for both Figs. 3 and 4; these density compression values are not on a linear scale.

The longitudinal sound speeds (Fig. 3a) and moduli (Fig. 4a) for $\langle 100 \rangle$ Al show a continual increase to ~ 120 GPa ($\sim 62\%$ percent compression) followed by a significant drop between 120 and 140 GPa before increasing again beyond 140 GPa. For $\langle 100 \rangle$, 120 GPa represents the onset

of melting and the increase beyond 140 GPa shows that the melting is complete at 140 GPa. Thus, ~20 GPa represents the mixed phase range for this orientation.

In contrast to the $\langle 100 \rangle$ results, the $\langle 110 \rangle$ results show that the longitudinal sound speeds (Fig. 3b) and moduli (Fig. 4b) increase continually only until ~100 GPa (~56 percent compression) followed by a drop. For $\langle 110 \rangle$, ~100 GPa represents the melting onset; however, the completion of melting is >163 GPa for this orientation. Thus, the mixed phase range for this orientation is greater than 63 GPa.

The result in Figs. 3 and 4 show that the melting threshold and the mixed phase range for the solid-liquid transition are significantly different for $\langle 100 \rangle$ and $\langle 110 \rangle$ orientations – a conclusive demonstration of melting anisotropy. To gain insight into the observed anisotropy, potential differences in the shocked state for the two orientations are considered next.

The shock compression results in Fig. 2 shows no anisotropy. This finding and previous results [67] showing that pure Al single crystals, irrespective of the crystal orientation, display extremely small elastic limits– negligible stress deviators compared to longitudinal stresses – lead to the following outcome. For both orientations, the difference between pressure (or mean stress) and the longitudinal stress is negligible, and a single $P - V$ curve can represent Al single crystal Hugoniot (shock compressed states). Because of this feature, single crystal (Fig. 2) and polycrystalline [52] shock compression results for pure Al are indistinguishable (within experimental uncertainty).

The other variable of interest for the melting transition is temperature. Since temperature measurements are lacking in shock compressed Al, we use theoretical developments to estimate temperatures along the Hugoniot (shock compressed states). The Al equation of state (EOS) has

been widely studied [54,56–63] and the paper by Sjostrom et al [62] provides, likely, the most comprehensive description of a multiphase Al EOS obtained from first principles; thus, Ref. 62 was used for temperature estimates under shock compression. Although the theoretical EOS developments utilized static compression and shock compression results on polycrystalline Al, the near-identical single crystal and polycrystal responses under shock compression make a good case for using the calculated temperatures from Ref. 62 for the present work.

Fig. 5 shows the calculated Hugoniot (shock response) and the melt curve from Sjostrom et al [62]– along with static pressure data [68–70] used to develop the theoretically calculated melt curve. The vertical lines denote the relevant pressures for melting onset and completion for the two orientations from the present work. Regarding Fig. 5, the following comments are noteworthy: (1) the calculated temperature (3352K) at ~100 GPa, the melting onset for <110> Al, is significantly below the calculated melt curve; the calculated temperature (4360K) at ~120 GPa, the melting onset for <100> Al, is also lower but the difference is not as significant; (2) regarding the temperatures for completion of melt, significant differences are again observed – the <100> results show considerably larger discrepancy with the calculated curve than the <110> results.

We note that the primary purpose of Fig. 5 is not to highlight quantitative differences between theoretical predictions and experimental results regarding the melt transition. Instead, the noteworthy finding is that the melting anisotropy observed in our experiments cannot be understood, even qualitatively, in terms of the usual $T - P$ melt curves. Hence, other differences in the shock compressed states for the two crystal orientations need to be considered.

In addition to a near-discontinuous change in temperature and pressure, shock wave compression (uniaxial strain) in crystalline solids leads to significant lattice deformation which, in turn, results in microstructural changes (formation of dislocations or stacking faults or twins) in

the shocked state – as has been well documented in both experimental [71–75] and theoretical [21,76] studies. We note that the dependence of microstructural changes (defect types and density) on the directionality of deformation in crystals is a well-established result of long standing in materials science [77]. A recent study [78] examined the microstructures in soft-recovered Al single crystals shock compressed along different crystal orientation and clear difference in dislocation densities were observed for $\langle 100 \rangle$ and $\langle 110 \rangle$ orientations. These results [78] demonstrate that shock wave induced uniaxial strain compression along two different crystal orientations result in different microstructures; thereby, providing a potential explanation for the observed melting anisotropy. However, we note that some caution is warranted regarding the results from Ref. 78, since the peak stresses examined (~ 9 GPa) were significantly lower than the peak stresses examined in this work (> 100 GPa). Whether these differences will persist beyond 100 GPa remains an open question.

The proposed link between microstructure and melting anisotropy is also well aligned with previous suggestions [5,79–81], unrelated to shock compression, that microstructural defects like dislocations can facilitate melting. A more recent theoretical study [82], also unrelated to shock compression, examined the role of defects on melting in copper and aluminum and makes a strong case that the role of microstructural defects – not included in classic melting theories – needs to be considered for evaluating competing pathways for melting. Extension of this approach [82] to shock compression would be desirable.

Since $T - P$ phase diagrams, central to melting transition studies, are determined primarily from static compression experiments [83] that do not involve deformation, deformation-induced microstructural defects are unlikely to contribute to the melt boundaries determined from such experiments. Thus, the use of $T - P$ phase diagrams from static compression studies for

experimental conditions that entail superposed deformation – geo/planetary sciences [84–86], high velocity impacts involving space and ballistic applications [87–90], and materials synthesis/fabrication involving deformation – needs to be viewed with caution. Although thermodynamic descriptions of melting in defected solids constitute a significant challenge [21], we hope that our results will motivate theoretical studies to undertake the requisite developments to incorporate the effects of temperature, pressure, and deformation-induced microstructure in modeling the melt transition – a ubiquitous structural change.

In addition to the theoretical developments noted above, experimental measurements are also needed to explicitly examine the mechanistic role of microstructural changes on shock-induced melting. Because sound speed measurements cannot address this need, in-situ measurements that can probe the microstructure in real time (e.g. x-ray diffraction on ns time scales) are needed to gain insight into the linkage between microstructural changes and melting.

Using sound speed measurements in Al single crystals shock compressed along two different crystal orientations, we have conclusively demonstrated the dependence of melting on crystal orientation. In addition to addressing a long-standing fundamental question in condensed matter physics, two broad attributes of the present findings are noteworthy. First, if melting anisotropy is observed in an extremely soft fcc crystal like Al, it is very likely that most other crystalline solids will display similar behavior. Second, under conditions involving superposition of temperature, pressure, and deformation, the role of deformation induced microstructure on the melting transition needs to be carefully assessed. Both of these attributes are expected to be relevant for conditions not involving plane shock wave compression utilized in our work. Theoretical and experimental developments, though likely to be quite challenging, are needed to understand the linkage between deformation induced microstructure and crystal melting because

of the fundamental aspect of this issue for understanding the melting transition [5,79–82] and the likely benefits for geophysical sciences [84–86], high velocity impacts involving space and ballistic applications [87–90], and materials related technologies involving material design and/or prediction of material response in various high-temperature applications such casting, welding and additive manufacturing.

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Figures and captions

FIG 1: Experimental configuration used for wave profile measurements in Al single crystals shock compressed along $\langle 100 \rangle$ and $\langle 110 \rangle$. Wave profiles were measured at the Al/LiF window interface using both VISAR (532 nm, green arrows) and PDV (1550 nm, red arrows) measurements. PDV data were also used to obtain shock wave arrival times at the Al buffer free surface.

FIG 2: Shock velocity – particle velocity (2(a)) and the equivalent stress – volume (2(b)) results for Al shock compressed along $\langle 100 \rangle$ (red points) and $\langle 110 \rangle$ (blue points); the black line (2(a)) is a linear fit to all the data presented in the figure. The solid symbols correspond to data obtained from the present work and the open symbols correspond to the reanalyzed results at lower stresses from Ref. 37.

FIG 3: Eulerian sound speed as a function of peak longitudinal stress in the shocked state (a) $\langle 100 \rangle$ orientation, (b) $\langle 110 \rangle$ orientation. The nonlinear scale on top of each plot shows the density compression obtained using the Hugoniot relations. Stress values indicated correspond to onset and completion of melting. For $\langle 110 \rangle$, completion of melting is greater than 163 GPa. Stress uncertainty is smaller than the symbol size.

FIG 4: Longitudinal modulus as a function of longitudinal stress in the shocked state (a) $\langle 100 \rangle$ orientation, (b) $\langle 110 \rangle$ orientation. The nonlinear scale shown on top of each plot corresponds to the density compression obtained using the Hugoniot relations. Stress values corresponding to melting onset are again indicated.

FIG 5: Temperature – Pressure phase diagram for Al [62]; symbols correspond to experimental data from static compression studies [68–70]; brown solid curve corresponds to the melt; black dashed line corresponds to the calculated Hugoniot for shocked Al [62]; red and blue vertical dash-dotted lines corresponds to onset and completion of melt from this study in shocked $\langle 100 \rangle$ Al and $\langle 110 \rangle$ Al, respectively. We note that melt completion for $\langle 110 \rangle$ is greater than 163 GPa. Temperatures shown are based on results from Ref. 62.

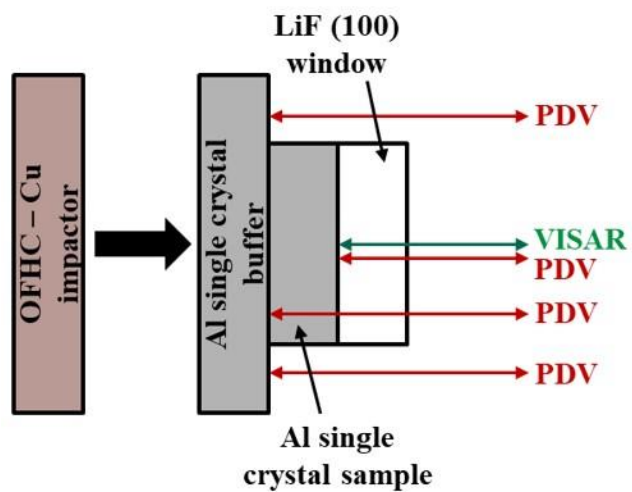


FIG 1

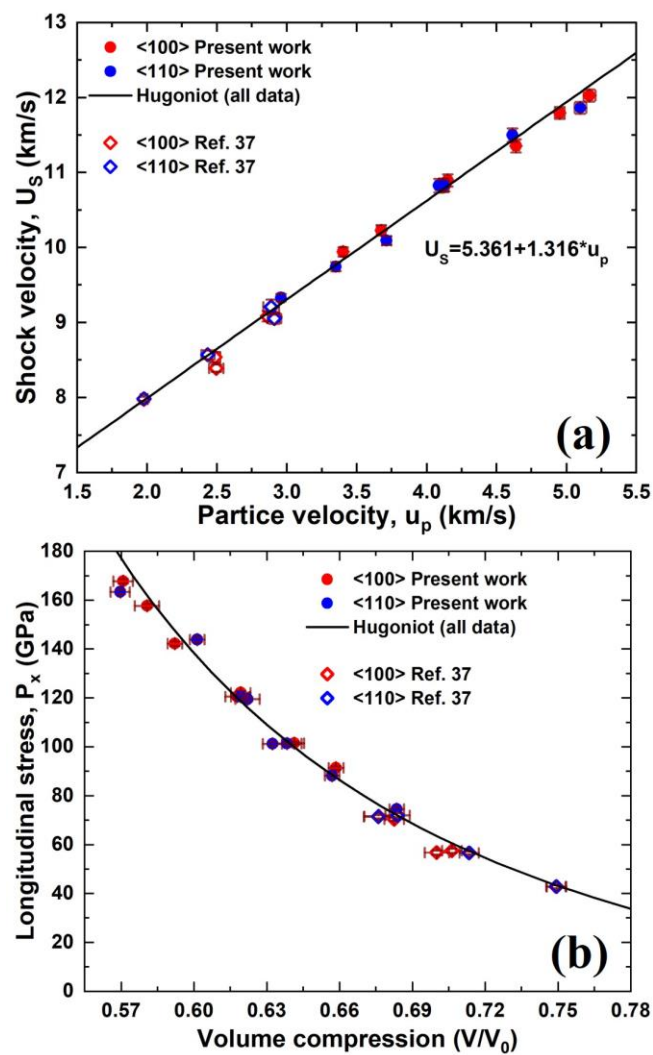


FIG 2

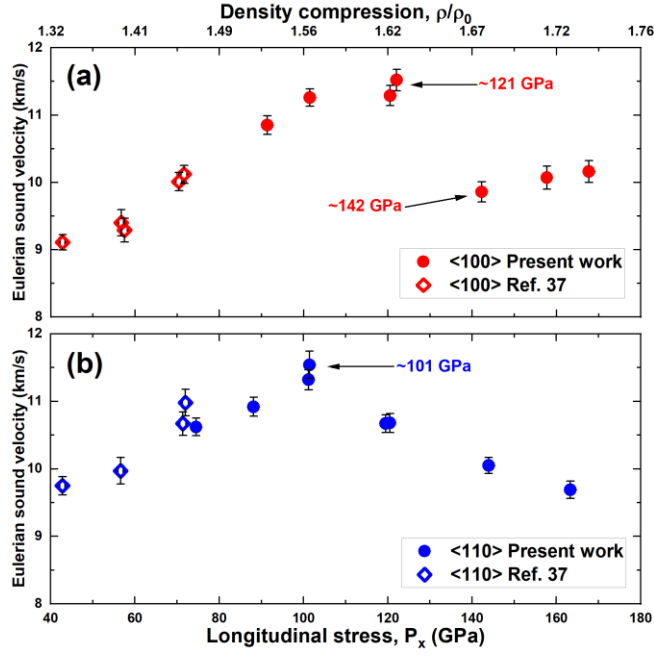


FIG 3

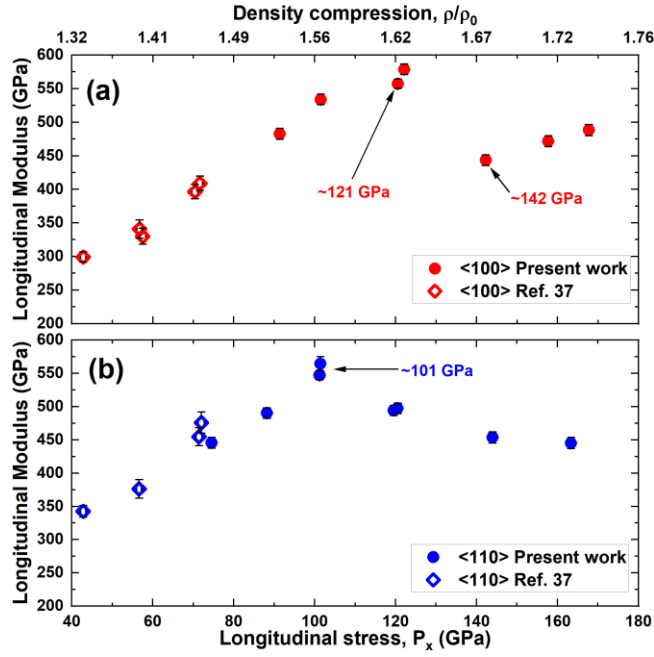


FIG 4

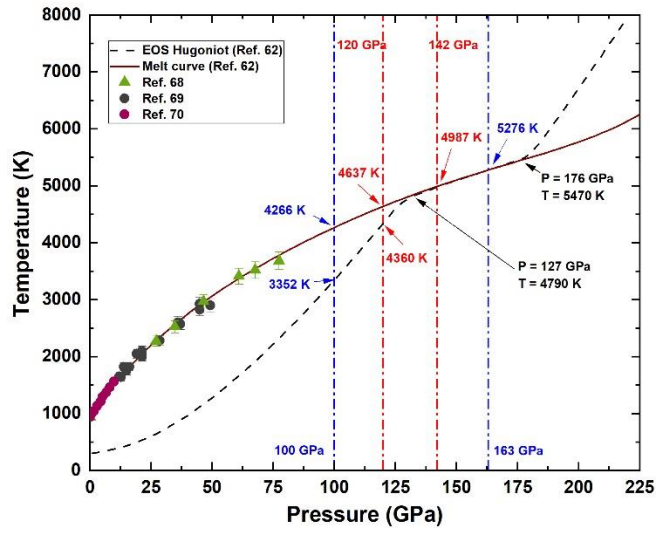


FIG 5