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# Atomistic simulations on the dynamic properties of shock and release melting in single crystal Al

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ABSTRACT

Molecular dynamics simulations are performed to investigate the dynamic properties of melting in single crystal Al under [0 0 1] shock loading and release. Our simulations suggest that the shock melting can be accompanied with shuffle mechanism and especially with collision cascade. The overheated interval and the relaxation of shear stress below and above shock melting pressure are presented by the microstructure and dynamic paths. The Hugoniot results can describe the shocked solid, liquid and also solid-liquid phases, and the range of shock melting pressure is about 125–155 GPa. From different release paths, we observe the transition from surface melting to sustained release meting. The shock pressure leading to melt at release is about 72 GPa. For higher shock pressure, the melting speed will keep some constant after the early nucleation. In fact, the release melting involve both the solid-liquid interface movement and the continuous nucleation in front of it. Finally, we present the different release *P-T* paths (solid-solid, solid-liquid and liquid-liquid) to show the difference of melting near and far away from the free surface.

## 1. Introduction

Shock-induced melting of metals has always been a significant concern in shockwave and high pressure physics. To this day, extensive experimental [1–5] and theoretical [6–12] investigations have been conducted on this solid to liquid transition. Among them, Al is a most important and widely studied material of shock melting. Early in 1972, Ahrens [1] presented the shock melting of multiple metals (Al, Fe, etc.) by measuring the entropy production in experiments of explosive in contact and flay-plate impact. In 1983, McQueen et al. [2] reported the Hugoniot pressure for the melting of 2024 Al, beginning at about 125 GPa and ending at about 150 GPa. Later, Chhabildas et al. [3] observed the continued reduction of the Al shear strength to zero with shock stress over 100–160 GPa because of shock melting occurrence, based on the wave profile measurements. In addition, De Rességuier et al.[5] found the melting of Al in their laser driven shock experiments, where they observed the liquid fragmentation state at the shock breakout pressure of 123 GPa. Although the shock melting pressure could be roughly determined according to the macroscopic profiles, how to explain and predict this phenomenon still requires more knowledge on the melting curves and melting process mechanism.

As a powerful supplement to the experiment, *ab intio* molecular dynamics (MD) simulations have attracted a growing interest in the calculations of high pressure melting. Based on density functional theory within the generalized gradient approximation, Bouchet et al. [6] simulated the melting curve of Al up to 300 GPa. It was found that the results from the two-phase approach are the closest to experiments. Ogitsu et al. [7] presented *ab initio* calculations of the linear optical conductivity of heated Al at ambient pressure and at the conditions relevant for shock melting (125 GPa, 5000 K), indicating that *in situ* measurements of optical constants are able to diagnose the shock melting of Al. Besides, a comprehensive analysis of available shock-wave data was conducted [9], where the agreement and discrepancies of simulation results with measurements were discussed. It demonstrates that the quantum MD method can be used for calibration of semi-empirical state equations in the absence of experimental data. In fact, various efforts have been put on the modelling on the shock melting to explain and determine the melting conditions. Such as the melting curve model of Al based on first-principles calculations developed by Moriarty et al.[10], which predicts the shock melting pressure begins at about 120 GPa and ends at about 155 GPa, and the shock-release model proposed by Dai et al. [12], which can be used to assess the melting on the principal Hugoniot, and to relate initial shock to release melting.

From the thermodynamic point of view, melting is a first-order phase transition that includes nucleation and growth stages. Within the

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classical approximation, MD simulations [13–20] are applicable to explore the melting process at nanoscale. For example, Jeong et al. [17] inferred that the Hugoniot melting of Al begins at 120 GPa and ends at 140 GPa, based on the static MD simulations on the melting curve and Hugoniot states for the solid and liquid phases. In another work [18], Gubin et al. still used the Hugoniostat technique to investigate the dependence of melting temperature on pressure. Their calculations show that the melting of Al occurs at shock pressure of 122 GPa, and the corresponding temperature is close to that in static conditions. In another work [19] the Hugoniot melting is found to begin at 93.6 GPa and end at 140 GPa, by comparing the Lindemann melting curve with the two Hugoniot curves for the solid and liquid phases. Also, the crystal defects can make the pressure and temperature increase slightly for the same dynamic loading. However, on the melting nucleation and growth under direct shock loading, there are still many aspects to be understood, including the nucleation structure and time, as well as its dependence on the loading rate and crystal defects.

In this work, we mainly discuss the nucleation process and some dynamic properties for both shock melting and release melting of single crystal Al by direct MD simulations. The microscopic views of melting behind the shock wave are demonstrated in detail. Our simulations indicate the possible shuffle mechanism and especially collision cascade before shock melting, and the temporal evolutions of stress and microstructure are comparatively analyzed. The range of shock melting pressure is about 125–155 GPa as for the potential [21,22] used here. As far, there are still fewer direct simulations on release melting of Al. Although a small amount of simulations on the release melting of Cu were reported [23,24], where the sustained release melting was presented and the release path were thought to be isentropic regardless of release melting. The release melting pressure can be determined by the release path and the melting curve. In an experimental work, Kanel et al. [25] investigated the release melting pressures of Al, Cu, Ti and Mo based on the surface reflectivity using a pulsed proton beam, where the release melting of Al was determined at a threshold pressure in the range of 62–65 GPa. In our simulations, the shock pressure of melting at release is about 72 GPa, which is a little higher than that experimental observation. Besides, we further analyze the transition from surface to release melting and the various release pathes. The solid-liquid interface movement and the continuous nucleation are also presented.

## 2. Computational details

The embedded-atom-method (EAM) potential developed by Mei and Davenport [21,22] is adopted here, in view of its advantage in describing the high pressure melting of Al[17], although the melting point at zero pressure (826 K) is a little less than the experimental value (930 K). The computational model consists of $45_x \times 45_y \times 200_z$ fcc cells, where $x$,$y$ and $z$ axes are respectively in the [100], [010] and [001] directions. The MD code used here is developed by ourselves. After a sufficient relaxation of this model at zero temperature and pressure in canonical and micro-canonical ensembles, the shock loading is performed in micro-canonical ensemble. The shock wave is introduced along the $z$ axis via a momentum mirror[26], which means an infinitely massive piston moving with a certain speed. Thus, it is the supported shock pulse. The release process is derived from the reflection wave of shock front from surface. In the $x$ and $y$ directions, periodic boundary conditions are applied to reduce the surface effects.

Under the above designs, a series of MD simulations are carried out by varying the piston velocity from 2.0 to 6.0 km/s, which cover the solid and melted states of Al after being shocked. As for the simulation results, both the microstructural evolutions and dynamic properties are analyzed. Firstly, the microstructural changes are identified by the centrosymmetry parameter (CSP)[27], whose computational formula is:

$$\mathrm{CSP} = \sum_{i=1,6} |\mathbf{R}_i + \mathbf{R}_{i+6}|^2. \tag{1}$$

$\mathbf{R}_i$ and $\mathbf{R}_{i+6}$ are the vectors corresponding to the six pairs of opposite nearest neighbors in the initial fcc lattice. In this work, that six pairs of neighbors is no more updated with time. Referring to this value, we can easily find out the elastic, plastic or disordering deformations. The disordering or melting state can be approximately identified by $\mathrm{CSP} > 32\text{Å}^2$, although there is a certain fluctuation at high temperature.

Besides, the radial distribution function (RDF) and the mean-squared-displacement are also calculated, in order to further identify the melting process. Also, the compressive stress tensor is calculated according to the virial formula[28,29]:

$$\sigma_{\alpha\beta} = \frac{1}{V}\left(\sum_i m_i v_{i\alpha} v_{i\beta} + \sum_i \sum_{i>j} r_{ij\alpha} f_{ij\beta}\right), \tag{2}$$

where $\alpha$ ($\beta$) denotes $x$,$y$ or $z$ axes, $m_i$ and $v_i$ represent the mass and velocity of atoms $i$, and $f_{ij}$ is the force between atoms $i$ and $j$.

Based on these basic computational data, we trace the time evolutions in any $x$–$y$ section. Moreover, the Hugonoit relation is derived from the simulations of various shock states, and the release paths are derived from the pressure and temperature profiles on the release. The release melting speed is analyzed by the increase of melting layer number. For convenience, the temperature in this paper is calculated by the transverse velocities:

$$T = \frac{1}{2Nk_B}\sum_{i=1}^{N} m_i (v_{ix}^2 + v_{iy}^2). \tag{3}$$

This is just to avoid the calculation error caused by the wave front. As for the thermodynamic equilibrium region behind shock wave, it is equivalent to the statistics from three directions. The temperature here is actually instantaneous, related to the dynamic process.

## 3. Results and discussion

### 3.1. Shock melting

Firstly, except for plastic deformation, we observe structural transition and collision cascade before shock melting with the increase of piston velocity. All the microscopic views are summarized in Fig. 1, where the atoms are color-coded according to the CSP and the red (over $32\text{Å}^2$) is identified to be melted zones or the free surface. At the piston velocity of 2.0 km/s, there appear a few Shockley partial dislocations and stacking faults on the close-packed planes as expected. Whereas, we also find the formation of hcp zones as a result of the shuffling mechanism of {111} planes, which can be seen clearly in Fig. 2(a). Here, we identify the hcp structure based on CSP and also observation of the

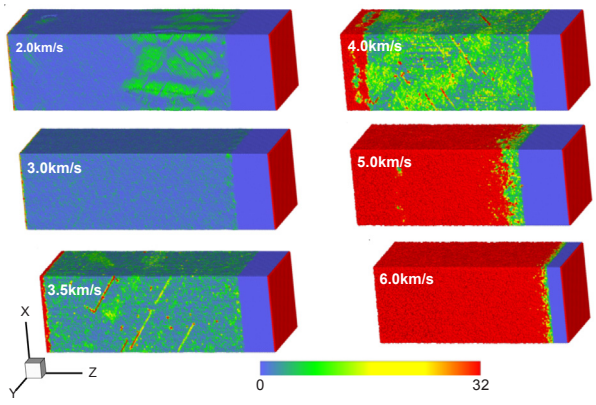


**Fig. 1.** Microscopic views of shocked samples at different piston velocities. Atoms are color-coded by the CSP. The structure transition ($U_p$ = 2.0 km/s), collision cascade ($U_p$ = 3.5, 4.0 km/s), and shock melting ($U_p$ = 5.0, 6.0 km/s) are all captured. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)