Plasticity-Mediated Structural Transformation of bcc Ta: Bridging Laser Heated Diamond-Anvil Cell and Shock Melting

CHRISTINE WU, PER SODERLIND, JAMES GLOSLI, JOHN KLEPEIS, Lawrence Livermore National Lab — Determination of the melting curve of a metal under high pressures is essential for establishing its phase diagram, and has wide scientific implications, including our understanding of the Earth’s interior. Currently, melting temperatures at high pressure are primarily measured by \textit{in situ} laser-heated diamond-anvil cell (DAC) or shock wave experiments. Often, but not always, these two methods yield significantly different results for metals with non close-packed structures, such as bcc metals. For instance, anomalously flat melting slopes were reported for numerous bcc metals by DAC. The flatness of the melting slope is in sharp contrast to the classical Lindemann behavior which shock-melting temperatures follow closely. In this presentation, we will report our finding of a plasticity-mediated structural transition of bcc Ta to a partially disordered glassy structure obtained from molecular dynamics (MD) simulations. This transition is fully consistent with reported DAC low melting, thus provide a highly probable resolution to the long-standing controversy in melting of metals under high pressures.

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