Abstract Submitted
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First-principles thermodynamics–specific heat of Mo from density functional theory molecular dynamics simulations ANN E. MATTSSON, THOMAS R. MATTSSON, Sandia National Laboratories, NILS SANDBERG, Royal Institute of Technology, Sweden, RICKARD ARMIENTO, University of Bayreuth, Germany — A fundamental understanding of thermodynamical properties like specific heat is necessary in order to model shock compression of condensed matter to high fidelity. It is therefore interesting that also central issues remain unsatisfactorily understood for technologically important body centered cubic metals like Mo. For example the long-standing question whether the strong increase of the specific heat of Mo close to the melting point is caused by a high (several percent) concentration of vacancies or by anharmonic lattice and electronic effects. Here we show, through density functional theory (DFT) molecular dynamics simulations of vacancy motion in Mo close to the melting point, using the new AM05 density functional, that a low (fractions of percent) concentration of vacancies does explain experimental observations of specific heat and self-diffusion. We furthermore quantify and discuss the origin of the anharmonicity as well as implications for modeling of shock-processes from an atomistic point of view. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

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