

Parallel codes for simulating elastic constants and melting in Ar and Mg

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Abstract

We have studied bulk and surface melting in Ar and Mg, using molecular dynamics codes that were parallelised with MPI and spatial decomposition. Optimal strategies to obtain the elastic constants needed to evaluate melting temperatures were first found for the simpler cubic system of Ar and then applied to the non-Bravais HCP Mg system. Excellent speedup was found for a reasonable number of processors, and values of elastic constants and shear moduli were in good agreement with experimental measurements. © 2010 Published by Elsevier B.V.

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1. Introduction

Melting is an everyday phenomenon whose explanation on an atomic scale has been in need of clarification. Adler, Polturak, Kanigel and Sorkin [1, 2] carried out studies of bulk and surface melting on several cubic lattices. Sorkin et al. [2] suggested that the Born criterion (melting is caused by a mechanical instability due to softening of the shear moduli [3]) can be extended to surface melting. Are these conclusions also valid for the non-Bravais HCP (hexagonal close packed) system? The absence of superheating of solids hints that their melting begins at a free surface. The formation of a thin liquid surface layer, which is observed experimentally, eliminates the barrier for nucleation of the liquid phase. Some claim that this phenomenon resembles wetting of the solid by its own melt.

In order to explore the question as to whether the Born criterion can be extended to the HCP lattice we have carried out Molecular Dynamics (MD) simulations of Mg both in the bulk and near surfaces in the three main HCP facet directions. Rather large samples were needed and thus we needed to move this project to a parallel code. In the next section we will describe our approach to measuring melting temperatures from softening of shear moduli, as well as algorithms for parallelizing such simulations with MPI. We will introduce these first for the simple case of cubic Ar and then present a discussion of the extension of this type of modelling to the more complex, non-Bravais HCP structure. Atomistic visualizations with AViz [4] were employed, both in the debugging phase and in order to understand the melting process.

2. Why we need to evaluate elastic constants - measuring the melting temperature

If an external force acting on a body or if one part of the body applies force on another part, it is said that the body is in a state of stress. Stress, σ , is defined in units of force, F , per unit area, A , as $\sigma = F/A$ and can be characterized in the general case by the stress tensor. Strain, ε , describes the state of deformation of a solid; there is dilatational strain which changes the volume, but not the shape and deviatoric strain which in contrast changes the shape, but not the volume.

For a field of deformations $\vec{u} = (x, y, z)$, we can define a symmetric strain tensor in the following way:

$$\varepsilon_{\alpha\beta} = \frac{1}{2} \left(\frac{\partial u_{\alpha}}{\partial x_{\beta}} + \frac{\partial u_{\beta}}{\partial x_{\alpha}} \right), \quad \alpha, \beta = 1, 2, 3, \quad (1)$$

where 1, 2, 3 replace the spatial coordinates x, y, z . Strain, is proportional to stress, according to Hooke's Law: $\varepsilon = S\sigma$ or $\sigma = C\varepsilon$ and is generalized for an anisotropic solid, in terms of tensors by

$$\varepsilon_{\alpha\beta} = \sum_{\gamma\delta} S_{\alpha\beta\gamma\delta} \sigma_{\gamma\delta} \quad \text{or} \quad \sigma_{\alpha\beta} = \sum_{\gamma\delta} C_{\alpha\beta\gamma\delta} \varepsilon_{\gamma\delta}. \quad (2)$$

The fourth-rank elasticity tensor $C_{\alpha\beta\gamma\delta}$ has $3 \times 3 \times 3 \times 3 = 81$ components, but due to symmetry the number of independent components is reduced to three in cubic type lattices and five in HCP lattices. Voigt notation reduces the number of indices:

$$\begin{aligned} 11 \rightarrow 1 &\Rightarrow C_{1111} \equiv C_{11}, \\ 22 \rightarrow 2 &\Rightarrow C_{1122} \equiv C_{12}, \\ 33 \rightarrow 3 &\Rightarrow C_{1133} \equiv C_{13}, \\ 23, 32 \rightarrow 4 &\Rightarrow C_{3223} = C_{2323} \equiv C_{44}, \\ 13, 31 \rightarrow 5 &\Rightarrow C_{3113} = C_{1313} \equiv C_{55}, \\ 21, 12 \rightarrow 6 &\Rightarrow C_{1221} = C_{2121} \equiv C_{66}. \end{aligned} \quad (3)$$

In this notation the elastic constants are written as C_{ij} where the new indices i and j will run over 1, 2, 3, 4, 5 and 6. The quadruple sum is replaced by a double sum. For cubic lattices the independent components of the elasticity tensor [1] are: C_{11}, C_{12} , and C_{44} and for HCP lattices [5] they are $C_{11}, C_{12}, C_{13}, C_{33}$ and C_{55} .

The elastic constants hint about the stability of a crystal by their relationship to the shear moduli which should be zero at the melting phase transition. According to Born [3] for cubic lattices the shear moduli are $2C' = C_{11} - C_{12}$ and C_{44} . For HCP lattices one obtains [5] $C_{11} + C_{12}, C_{11} - C_{12}, 2C_{55}$ and $0.5C_{33}$.

Calculation of these elastic coefficients is important for studying the melting transition and their elucidation from fluctuation formulas obtained by Ray and Rahman [6] and is commonly carried out in two steps. The first is to find the zero-stress reference matrix for the computational cell, H_0 , and the second is to run the NVT MD simulation to calculate the elastic coefficients. These calculations are time consuming and hence a parallel code is desirable. Full details for the Ar case are in [7] and for the Mg case in [8] and in a manuscript in preparation [9].

3. Parallel code for evaluating elastic constants for Ar with a cubic structure

All our calculations were made on NANCO, a 128 dual-core processor (2.2GHz AMD Opteron) with a VOLTAIRE interconnect based on DDR Infiniband [10]. In order to explore parallelization

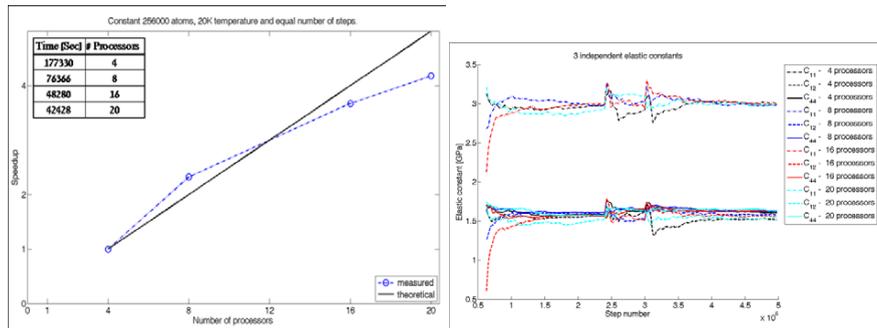


Figure 1: (left) Speedup as a function of no. of processors for Ar. (right) Several elastic constants of Ar measured for different numbers of processors. The jumps occur when some values are reset to give clearer results.

algorithms, simple, cubic argon systems with Lennard Jones (LJ) potentials and some 250,000 (equivalent to a 21.6nm sample) to just over one million (1,048,576, equivalent to 34.56nm) atoms were studied. We used the predictor corrector method to solve the equations of motion in an NVT ensemble with a Nose-Hoover thermostat. The sample was divided into slices and 4 stages of updates were made. First even numbered processors sent clockwise updates, then odd-numbered ones did so, next the even numbered ones sent counterclockwise updates and finally the odd-numbered ones did so as well. This minimised communication jams.

Speedup for the 250,000 atom sample is shown on the left of Figure 1. A run that took 177,330 seconds for 4 processors, took only 76,366 for 8 processors and 16(20) processors had times of 48280(42428)seconds. For larger numbers speedup was not as good and so we concluded that 16-20 gave an optimal number of processors to get good parallelization and a less than 24 hour turnaround.

The time development of the elastic constants is shown for several cases and processor numbers on the right of Figure 1. Our values are of the same order of magnitude as the experimental ones, for example at 20K results for C_{11} , C_{12} , and C_{44} , were 3.01/4.20, 1.51/1.81 and 1.61/1.54 for simulation/experiment and at 30K 2.98/4.00 1.59/1.80 and 1.64/1.45. Deviations may be due to this fluctuation based approach, but probably are mainly caused by the fact that while the LJ potential is better for Ar than for say a metal, it is not a perfect fit.

4. Parallel code for magnesium with a HCP lattice

A similar type of spatial decomposition was made for the Mg (HCP lattice) with the speedup as shown on the left of Figure 2, again with some 20 processors being optimal for reasonable turn around and utilization of resources. In this case both the lattice structure and the potential were far more complicated. Since magnesium is a metal we needed to use an Embedded Atom (EAM) potential, (which has an additional many-body interaction) and selected that developed by Sun et al. [11] from fitting to both experimentally measured properties and to others calculated from first principles. These include properties of both crystalline and liquid bulk phases, including the melting temperatures for HCP and metastable BCC solids. The potential is an extension of earlier work by Liu et al. [12] who developed an EAM potential for Mg by employing the force-matching method. The improvement in the work of Sun et al. compared with Liu et al. is that

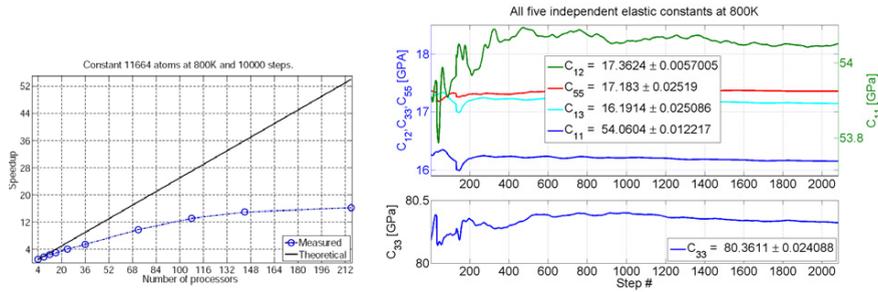


Figure 2: (left) Speedup as a function of no. of processors for Mg. (right) Variation of all five independent elastic constants with time for Mg.

Liu's potential gives rise to an HCP-BCC transition upon heating at zero pressure, such that the coexistence between HCP Mg and the liquid phase at the HCP melting point is metastable. Such metastability can potentially lead to artifacts in simulating melt coexistence and crystallization kinetics. In Sun's potential this problem was corrected and it gives rise to stable coexistence between the HCP crystal and its melt. (It may appear inconsistent to use a potential developed by fitting to the melting temperature to calculate it, but this provided validation to continue on to studying the melting temperatures in the different surface facet directions.)

The time development of all five elastic constants at 800K is shown on the right of Figure 2. These results led to shear moduli that have the same form of behaviour as a function of temperature to experimental measurements, but a consistent, small, systematic gap in values. The shear moduli collapsed as predicted at the melting temperature. In Figure 3 we show initial and final images of a sample near the melting temperature, prepared with AViz. Note how initially layers are colored according to a position related color code. Each atom retains its initial color throughout the simulation and near melting we can observe the layer mixing. Details of this study and its extension to surface melting on the main HCP facets will be discussed in a forthcoming longer paper, [9]. In brief, we found that for the closest packed facet a quasiliquid appeared just before the sample collapsed and for the loosest packed one it appeared more gradually. Comprehensive analyses of the extensive numerical data including RMS vibration amplitudes, local density profiles, and of the change in the lattice spacing near the surface will also be presented in [9].

5. Discussion

Use of the parallel algorithm turned otherwise impossible into possible and both visual and numerical results strongly confirm that the Born criterion is valid for both bulk and surface melting on the HCP lattice. Good agreement with experimental measurements for elastic constants and shear moduli has been found. As will be presented in [9] our estimates of defect energies are also in excellent agreement with laboratory experiments.

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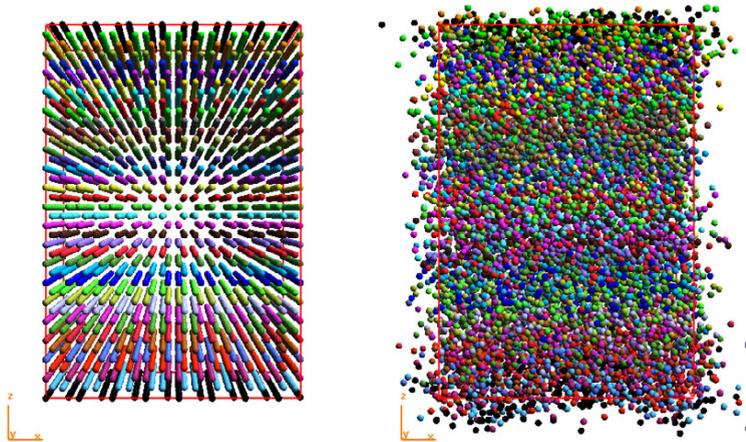


Figure 3: Snapshots of Mg during the heating process. The initial state is on the left, with atoms color coded according to original position and the final state on the right, with each atom retaining its initial color to show how the layers mix.

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