Implementation of an Augmented Tersoff Potential for the Modeling of the Phase-Change Material Germanium Telluride

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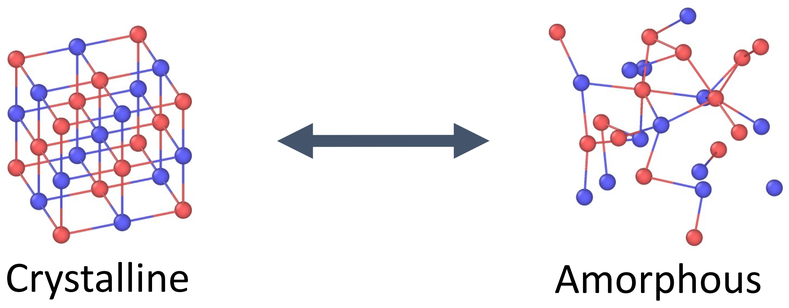
Introduction

Phase-change materials offer many promising applications due to their ability to switch between the crystalline and amorphous phases quickly.



Crystalline Amorphous

The drastically different properties between these phases have been exploited in Blu-Ray and non-volatile memory technologies. However, research into these materials is still lacking due to the complex quantum phenomena that contribute to their unusual dynamics. Currently, the primary method for the study of these materials is to use the computationally expensive “ab-initio” simulation.

More efficient, classical models of these materials are necessary to characterize their dynamics at longer timescales. Here, we implement an augmented Tersoff potential into the open-source, molecular dynamics code LAMMPS to allow for large-scale, parallel simulations of the phase-change material germanium telluride.

Methods

The Tersoff potential described in this poster is a derivative of the potential proposed by Zipoli and Curioni [1]. This style of potential includes both two and three-body interactions, the latter of which is required to properly describe strongly covalent systems. The potential is defined as the following:

$$V_{ij} = f_c(r_{ij})[A_{IJ}e^{-\lambda_{IJ}r_{ij}} - b_{ij}^{IJ}B_{IJ}e^{-\mu_{IJ}r_{ij}}]$$

where,

$$b_{ij}^{IJ} = \chi_{IJ}[1 + (\beta_I\xi_{ij}^{IJ})^{n_I}]^{\frac{-1}{2n_I}}$$

$$\xi_{ij}^{IJ} = \sum_{k\neq i,j} f_c(r_{ik})e_{ijk}^{IJK}t_{ijk}^{I}$$

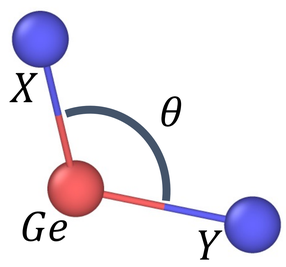
$$e_{ijk}^{IJK} = \exp(\mu_{IJ}r_{ij} - \mu_{IK}r_{ik})$$

$$t_{ijk}^{I} = 1 + \frac{c_I^2}{d_{IJK}^2} - \frac{c_I^2}{d_{IJK}^2 + [h_{IJK} - \cos(\pi\frac{\theta_{ijk} - \theta_{0,I}}{\pi - \theta_{0,I}})]^2}$$

Each equation varies from the standard Tersoff potential. For example, the addition of the secondary characteristic length term μ_{IK} provides a more accurate effective coordination number. The addition of $\theta_{0,I}$ and the terms d_{IJK}, h_{IJK} provide a better description of the angle distributions. Each system in this poster contains 1728 particles and is initially equilibrated at 1150K for 100 picoseconds. The 300K simulations are subsequently quenched to 300K over 100 picoseconds before their structural data is extracted. Each graph is an average over 6 separate runs, each from a different initial configuration, and is verified against ab-initio simulations based on density-functional theory.

Results & Conclusions

The results of our implementation are in good agreement with ab-initio data from Sosso et al. [2]. Two styles of comparisons of our work are depicted to the right. Bond angles, with X-Ge-Y illustrated here,



can be measured as a probability distribution (figures 1 and 3, 1150K and 300K respectively) and are good indicators of the accuracy of our model. To the right of the bond angles are the corresponding partial pair-correlation functions. These describe the density distribution of pairs as a function of radius. In each graph, our data is represented as the solid blue line and the ab-initio data by the dotted black line. A noticeable defect in our results is a higher peak in the Ge-Ge pair correlation functions at both 300K and 1150K.

These results demonstrate that a classical model, including both two and three-body interactions, can accurately model phase-change materials such as germanium telluride. Although this potential does not reproduce ab-initio results to perfection, further work will help refine defects.

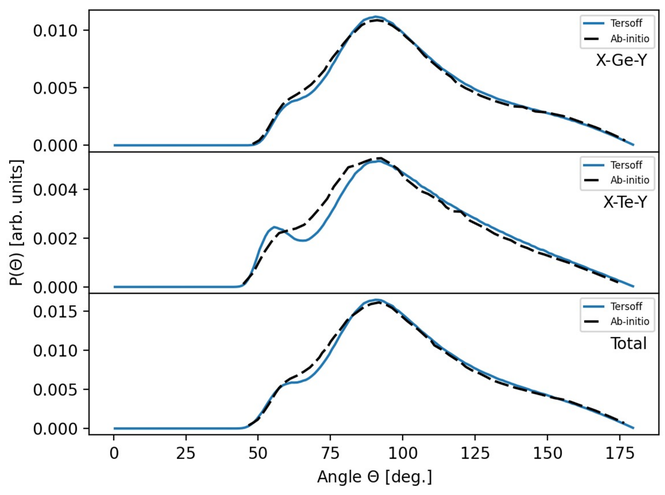


FIG. 1. Total and partial angle distributions, $\mathrm{P}(\theta)$, of triplet pairs X-Ge-Y and X-Te-Y at 1150K.

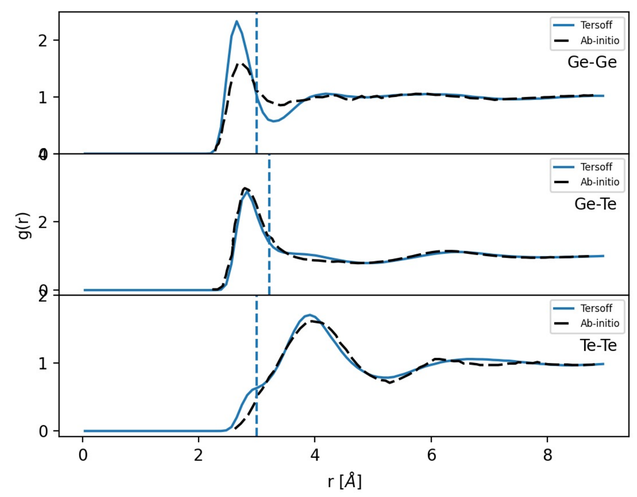


FIG. 2. Partial pair-correlation functions at 1150K. The vertical dotted line indicates the cutoff threshold for the bond angle distribution.

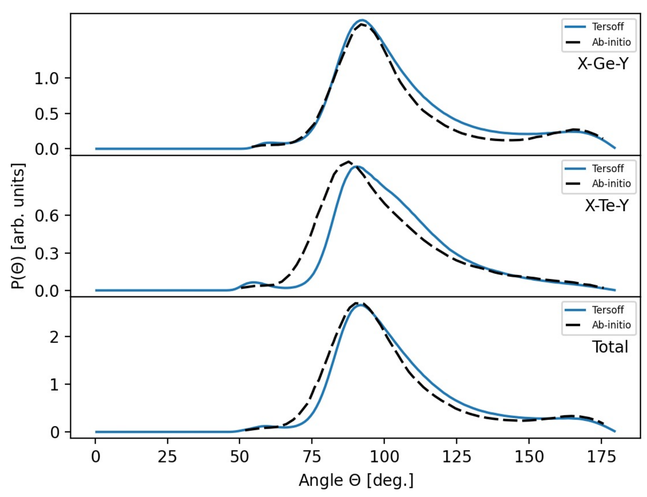


FIG. 3. Total and partial angle distributions, $\mathrm{P}(\theta)$, of triplet pairs X-Ge-Y and X-Te-Y at 300K.

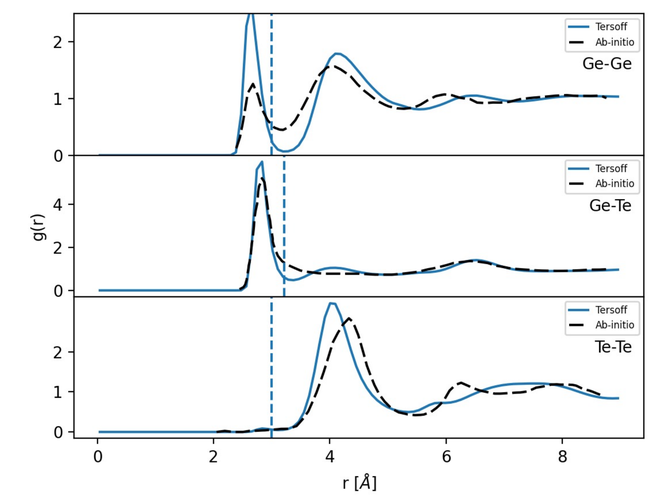


FIG. 4. Partial pair-correlation functions at 1150K. The vertical dotted line indicates the cutoff threshold for the bond angle distribution.

Further Work

The Tersoff potential implemented in this poster includes an additional coordination dependent term:

$$E_i^c = c_{I,1}\Delta z_i + c_{I,2}\Delta z_i^2$$

where,

$$\Delta z_i = \textstyle\sum_{j\neq i} f_c(r_{ij})b_{ij}^{IJ}$$

and $f_c(r_{ij})$ is a cutoff function and b_{ij}^{IJ} includes the effective coordination number. In the present work, this term is not implemented, however, this will be the focus of following efforts. Initial results indicate that this will contribute to correcting the increased first peak in the Ge-Ge pair correlation function.

Acknowledgments

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[2] Sosso G. C., Miceli G., Caravati S., Behler J. and Bernasconi M. 2012 *Phys. Rev. B* **85** 174103
[3] Plimpton S. Fast Parallel Algorithms for Short-Range Molecular Dynamics 1995 *J. Comp Phys* **117**, 1-19
[4] A. Stukowski 2010, Modelling Simul. Mater. Sci. Eng. 18,