

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Polyamorphism in tetrahedral substances: similarities between silicon and ice¹ ALEX ANTONELLI, Universidade Estadual de Campinas, KARL GARCEZ, Universidade Federal do Maranhao — Tetrahedral substances, such as silicon, water, germanium, and silica, share several thermodynamical anomalies. Among them, the so-called polyamorphism, i.e., the existence of more than one amorphous state, is, perhaps, the most studied one. In this work, we study the transformations between amorphs of silicon using Monte Carlo simulations. The simulations indicate that by compressing the low density amorphous state (LDA), which is obtained by quenching the liquid at high temperature, a new denser amorph is found [1]. The transformation between these two forms of amorphous silicon displays clear hysteresis, similar to the experiment reported by McMillan *et al.* [2]. However, analogously to the case of ice, our simulations indicate that upon annealing the unannealed high density amorphous silicon (uHDA) evolves to more stable forms. The annealing of uHDA at pressures on the order of 20 GPa gives rise to an even denser form, the very high density amorphous silicon (VHDA), while at much lower pressures, about 5 GPa, the uHDA transforms into a lower density form, the expanded high density amorphous silicon (eHDA). [1] K. M. S. Garcez and A. Antonelli, *J. Appl. Phys.* **115**, 063504 (2014), [2] P. F. McMillan *et al.*, *Nature Mater.* **4**, 680 (2005).

¹Work supported by FAPESP, CNPq, CAPES, and FAEPEX/UNICAMP

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Date submitted: 13 Nov 2014

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