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***Ab initio* molecular dynamics study of pressure-induced amorphization in sulfur¹**

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We report results of *ab initio* constant-pressure molecular dynamics simulations of sulfur compression leading to structural transition and pressure-induced amorphization [1]. Starting from the orthorhombic S-I phase composed of ring molecules we find at room temperature and pressure of 20 GPa a transformation to monoclinic phase where half of the molecules develop a different conformation. Upon further compression, the monoclinic phase undergoes pressure-induced amorphization into an amorphous phase, in agreement with experiments [2,3]. We further study the dynamics of the amorphization transition and focus on the evolution of intra and intermolecular distances in the monoclinic phase in order to provide a microscopic insight into the rings disintegration process leading to amorphization. In the amorphous form we examine the structural properties and discuss its relation to the experimentally found amorphous form as well as to the underlying crystal phases. The amorphous form we find appears to correspond to the experimentally observed low density amorphous form [3].

[1] Dušan Plašienka and Roman Martoňák, Phys. Rev. B, 094112 (2012)

[2] H. Luo and A. L. Ruoff, Phys. Rev. B, 569 (1993)

[3] C. Sanloup, E. Gregoryanz, O. Degtyareva, and M. Hanfland, Phys. Rev. Lett., 075701 (2008)

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