Ab initio prediction of the incongruent melting relation in the $MgO-SiO_2$ system at multi-megabar

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Magnesium silicates are thought to be the major components of the mantle of terrestrial planets and the core of giant planets (Guillot, 1999; Seager *et al*., 2007). However, the thermodynamic phase equilibrium in the $MgO-SiO_2$ system is still not well studied at multi-megabar, including melting relations. A recent laser shock experience reported two discontinuous phase changes in $MgSiO_3$ at 300-400 GPa (Spaulding *et al*., 2012), but an *ab initio* molecular dynamics study identified no clear transition in $MgSiO_3$ liquid (Militzer, 2013). Boates and Bonev (2013), on the other hand, examined a decomposition reaction of liquid $MgSiO_3$ into solid MgO and liquid SiO_2 and reported that liquid $MgSiO_3$ is dissociated at ~300 GPa. This result implies a possible incongruent melting. However, the reaction they considered is too simple and unrealistic. The detailed phase diagram in the $MgO-SiO_2$ system is therefore required to be clarified at multi-megabar. In this study, we perform *ab initio* free energy calculations based on the thermodynamic integration method (Kirkwood, 1935) and determine the melting phase relation in this binary system.

Keywords: ab initio calculation, MgO-SiO2 system, incongruent melting, multi-megabar

