

## **A simulation study of induced failure and recrystallization of a perfect MgO crystal under non-hydrostatic compression: Application to melting in the diamond-anvil cell**

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### **ABSTRACT**

Recent experimental studies revealed that the thermal pressure in a diamond-anvil cell with laser heating can be large. Accounting for this pressure is therefore important for treatment of experimental results. In earlier studies, we developed an MgO model that was demonstrated to perform very well for calculations of thermoelastic properties. Here, we study the effect of thermal stress on the behavior of MgO under high pressure and temperature conditions using molecular dynamics and the earlier developed interatomic potential. The simulations show that thermal stress can produce such effects as dynamic recrystallization, which may be interpreted as onset of convective-like motion and which may cause a change in the slope of laser power-temperature curve. Because these two criteria are used for the identification of melting, it is possible that what was interpreted as melting in previous experiments with MgO was in reality recrystallization.