INFRARED ABSORPTION OF MGO AT HIGH PRESSURES AND TEMPERATURES: A MOLECULAR DYNAMIC STUDY.

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Abstract

We calculate by molecular dynamics the optical functions of MgO in the far infrared region 100-1000 cm(-1), for pressures up to 40 GPa and temperatures up to 4000 K. An ab initio parametrized many-body force field is used to generate the trajectories. Infrared spectra are obtained from the time correlation of the polarization, and from Kramers-Kronig relations. The calculated spectra agree well with experimental data at ambient pressure. We find that the infrared absorption of MgO at CO(2) laser frequencies increases substantially with both pressure and temperature and we argue that this may explain the underestimation, with respect to theoretical calculations, of the high-pressure melting temperature of MgO determined in CO(2) laser-heated diamond-anvil cell experiments.