

Photoelasticity of Crystalline and Amorphous silica from First Principles

Davide Donadio^(a), Marco Bernasconi^(a), Francesco Tassone^(b)

^(a) Dipartimento di Scienza dei Materiali and Istituto Nazionale di Fisica per la Materia, Universita' di Milano-Bicocca, Via Cozzi 53, Milano, Italy

^(b) Pirelli Cavi e Sistemi S.p.a., Viale Sarca 222, Milano, Italy

Based on density-functional perturbation theory we have computed from first principles the photoelastic tensor of few crystalline phases of silica: quartz, α -cristobalite, β -cristobalite at normal conditions and at high pressure. Agreement with available experimental data is within 10-15 % as expected from the overestimation of the dielectric constant within the local-density approximation to the exchange and correlation energy. The photoelastic tensor of models of amorphous silica (up to 162 atoms large) is also computed and compared with experimental data. A phenomenological model suitable to describe the photoelastic properties of different silica polymorphs is devised by fitting on the ab-initio data.