Séminaire de Chimie Théorique

Salle Conférence, 3eme Est, bat. A12

Mercredi 8 Mars à 14:00

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Glass properties enhancement by mean of ion implantation: A theoretical study.

Ion implantation has been wildly used by the industry since the beginning of the 70th to dope semi-conductors for micro-electronics applications, and more recently for surface treatment of materials such as metals, polymers and elastomers. This technique consists in bombarding under vacuum a substrate with high energy ions (50-200keV). The ions violently penetrate the surface of the material and then are slowed down by a complex energy loss mechanism involving inelastic (electronic stopping) and elastic collisions (nuclear stopping). Apart from the type of implanted ions (C, N, O, Ar), ion implantation relies on two parameters: the dose and the tension. They respectively control the amount of implanted species and the implantation depth. The latter also depends on the charge (+1, +2, +3, …) of the implanted species, as the charge state affects the energy of the ions. Upon ion implantation, the structure, composition and nature of the surface of a material are strongly modified, directly affecting its properties.

The modelling of a glass is a complex task as it is a disordered material typically characterized by a rich chemical composition (mixture of oxides). Its disordered aspect imposes to work with large simulation cells, and to reproduce its composition is challenging as it requires setting up the methods at both quantum-chemistry (basis sets and pseudo-potentials) and force field (force field parameters) levels. Modelling an implanted glass is actually even more delicate. In the case of nitrogen implantation, for a typical dose of 10^{16} ion/cm^2 and a tension of 35 keV, the surface composition is greatly modified up to 300 nm in depth, where nitrogen species are still detected. Thus, modelling a system with such a long range concentration profile is very challenging as it would impose to work with huge 2D simulation cells. Moreover, as the charged state of the implanted species after implantation is unknown, these simulation cells would have to be treated at the quantum chemical level that can account for charge fluctuations.

To get insight on the effect of nitrogen implantation on the electronic structure and hardness of a glass, we first focus on silicon dioxide (SiO_2) as a model case. We investigated the effect of ion implantation on the density of states and stiffness coefficients of crystalline and amorphous SiO_2, varying the implantation site (substitutions/insertions), as well as the net charge of the system (0, +1, +2, +3) to simulate the implantation of different charged species (N, N^+, N^{++}, N^{+++}). Then we investigated the effect of the surface composition of implanted and non-implanted soda lime glasses on the hardness of the material. Our calculations support the hardness enhancement observed experimentally by our industrial partner (AGC).

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