Neutron diffraction and computer simulation studies on the plastic phase of C_2Cl_6

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Hexachloroethane (C_2Cl_6) is an interesting material with three different solid phases[1](orthorombic between 4 and 318K, monoclinic between 318 and 344K and a plastic phase (BCC) stable from 344K up to the melting temperature, 458K). In plastic or orientationally disordered phases[2] molecules conserve the translational order but they lose the orientational one, as can be seen from Fig. 1.

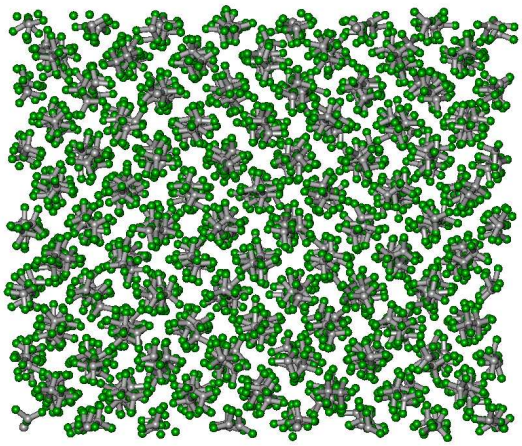

FIG. 1. Snapshot of an MD configuration of the plastic phase of C_2Cl_6.

In this contribution we report results (simulation and experiments) on the structure of C_2Cl_6 in the range of temperatures of the BCC phase (345-450K). Neutron diffraction experiments were carried out at the diffractometer dedicated to glasses and liquids D4c[3] at the Institute Laue Langevin (ILL, Grenoble, France). Molecular dynamics (MD) simulations were performed using the Gromacs[4] package. The potentials parameters were chosen from the Gromos53a6[5] forcefield. The simulations were carried out in the NPT ensemble using: $\Delta t = 2$fs, shifted cut-off from 16 to 17 Å for Lenard-Jones interactions and 20Å for coulomb pairs. We used the Particle-Mesh-Ewald method to deal with the long-range electrostatic forces. The system box contained 2000 molecules. Each run was extended up to 500 ps and properties were obtained from the last 300 ps. We compare the static structure factor resulting from MD with neutron scattering experiments at T = 400K in Fig.2.

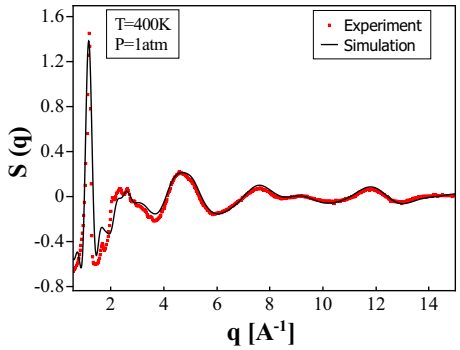

FIG. 2. Comparison between experimental (dots) and MD simulation (solid line) static structure factor at T = 400K and P = 1atm

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