o.m10.o5 Diffuse scattering of the plastic phase of solid Oxygen: from experiments to molecular dynamics.
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The plastic phase of molecular oxygen with its A15 structure and 8 molecules per unit cell possesses a non trivial orientational disorder with two sites of distinct symmetries. Although difficult to grow as a large monocrystal, experimental diffuse neutron scattering data have been obtained on single crystals. Due to the diatomic character of O_2 molecules, the contributions to the diffuse scattering signal arising from intramolecular and intermolecular correlations can be clearly separated — this is not the case for more complex systems. Simple statistical models can thus be developped analytically up to a certain extent to help to directly understand the nature of the statistical disorder at the atomic level. These insights can then be made more precise and/or slightly corrected thanks to molecular dynamics [1].

The total diffuse scattering signal is computed in order to compare with the experimental one. It is also computed through its various physical contributions. Analyses of the microscopic mechanisms at the molecular level are simultaneously performed in real space.

The complementarity between these two approaches, in reciprocal and in real spaces is discussed. The progression from simple, visualisable, analytic calculations to MD analyses is also shown to be important. This leads to a real understanding of the dynamics, more satisfying than a method based on a pure fitting process.

Notes

[1] F. Dunstetter, O. Hardouin Duparc, V.P. Plakhty, J. Schweizer, and A. Delapalme, Low Temp. Phys. **22(2)** (1996) 101, Fiz. Nizk. Temp. **22(2)** (1996).