Influence of thermal lattice vibrations on the visibility of GIFAD patterns

M S Gravielle *

Instituto de Astronomía y Física del Espacio (IAFE, UBA-CONICET), Buenos Aires, C1428EGA, Argentina

Synopsis We study the influence of thermal lattice vibrations on the visibilty of the interference structures present in the projectile distributions produced by grazing fast atom diffraction (GIFAD). For a LiF(001) surface in thermal equilibrium, GIFAD spectra are evaluated within the *Phonon- Surface Initial Value Representation* (P-SIVR) approach, which takes into account the vibrational modes of the crystal lattice. It is found that, even at room temperature, the relative intensities of the Bragg peaks are affected by the phonon contribution, this fact being relevant for surface analysis.

Nowadays GIFAD is considered as a sensitive tool for surface studies, which provides detailed information about the topmost atomic layer of the crystal. In particular, GIFAD experiments have been used to determine structural parameters of insulator surfaces, like rumpling, which are smaller than the vibrational amplitudes of the surface ions. But in most of these articles, thermal effects at room temperatue were evaluated through averaged corrections [1].

Since surface analysis with the GIFAD technique is usually based on the experimental-theoretical comparison of the relative intensities of the interference maxima, in this work we study the effect of thermal vibrations on such intensities as well as on the visibility of the diffraction peaks.

The contribution of thermal lattice vibrations into GIFAD projectile distributions is here investigated by means of a semi-quantum formalism named *Phonon- Surface Initial Value Representation* (P-SIVR) approximation. This method, based on the SIVR approach [2], describes the scattering with a harmonic crystal, involving phonon excitations. The first-order term of the P-SIVR transition amplitude, which corresponds to the elastic collision process (i.e., zero-phonon transition), can be expressed as a time integral that includes the Debye-Waller factor as a function of the momentum-transfer vector.

In Fig. 1 the P-SIVR distribution for 300 eV Ne atoms elastically colliding with a LiF(001) surface along the <110> channel is compared with the spectrum for an static crystal, derived within the SIVR approach. It is observed that not only the rainbow maxima, corresponding to the outermost peaks, are attenuated by the Debay-Waller factor. Also the relative intensities of Bragg peaks, whose angular positions are indicated with vertical lines, are strongly modified by the phonon effect. This behavior depends on the normal energy $E_{\perp}$ associated with the motion perpendicular to the incidence channel.

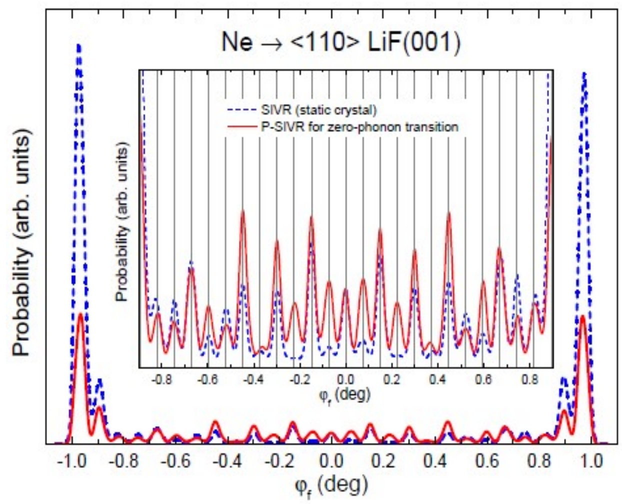

Figure 1. GIFAD distribution for Ne scattering from LiF(001) at room temperature, as a function of the azimuthal angle φ_f, for $E_{\perp}$= 0.3 eV.

Present results contribute to the understanding of the role of lattice vibrations in GIFAD. In addition, highest orders of the P-SIVR approach can be applied to deal with inelastic collisions involving phonon excitations, which is the subject of recent articles [3].

References

[1] Schüller A *et al* 2010 *Phys. Rev. A* **82** 062902

[2] Gravielle M S *et al* 2014 *Phys. Rev. A* **90** 052718

[3] Roncin P *et al* 2017 *Phys. Rev. B* **96** 035415

* E-mail: msilvia@iafe.uba.ar