

Energy-loss contribution for fast He atoms axially scattered off a silver surface

C.A. Ríos Rubiano^{*1}, G.A. Bocan[†], J.I. Juaristi^{#,‡}, and M.S. Gravielle^{*}

^{*} Instituto de Astronomía y Física del Espacio (IAFE, CONICET-UBA), Buenos Aires, Argentina

[†] Centro Atómico Bariloche and CONICET, S.C. de Bariloche, Río Negro, Argentina

[#] Depto. de Física de Materiales, Facultad de Químicas, UPV/EHU, 20018 San Sebastian, Spain

[‡] Donostia International Physics Center (DIPC) and Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), 20018 San Sebastian, Spain

Synopsis Angle- and energy-loss- resolved distributions for He atoms axially scattered off a Ag(110) surface are calculated in order to study the influence of inelastic processes on fast atom diffraction (FAD) spectra. Final projectile distributions are evaluated within a semi-classical formalism that includes dissipative effects due to electronic excitations. For monoenergetic beams the model predicts the presence of multiple peaks in energy-loss spectra. But these structures disappear when the experimental conditions are included, giving rise to an energy-loss distribution in good agreement with available experimental data. The inelastic contribution to FAD patterns is estimated.

Grazing-incidence fast-atom diffraction (GIFAD or FAD) on crystal surfaces has recently emerged as a powerful surface analysis method that allows one to probe surface interactions with an exceptional sensitivity. It is possible to observe FAD patterns for a wide variety of materials, even for metals where inelastic electronic processes are expected to play an important role against coherence. The aim of this work is to study the energy lost by swift He atoms after grazingly impinging on a Ag(110) surface, under the same conditions for which FAD has been observed [1].

We build the three-dimensional potential energy surface and charge density of the He-Ag(110) system from DFT calculations using the Quantum Espresso code. Angle- and energy-loss-resolved distributions of inelastically scattered projectiles are evaluated within a semi-classical formalism that includes dissipative effects due to electron-hole excitations through a friction force [2].

For incidence along different axial channels with a given impact energy, the model predicts the presence of multiple maxima in the energy-loss spectrum [3]. These structures are related to trajectories that probe different regions of the surface electron density. Such energy-loss peaks are however completely washed out when the experimental dispersion of the incident beam is taken into account, as shown in Fig. 1.

Present results (Fig. 2) suggest that the incoherent electronic excitations do not affect the relative intensities of internal FAD maxima, even though the total inelastic contribution to the momentum distribution is estimated around 75% for incidence along the [1-10] channel [3].

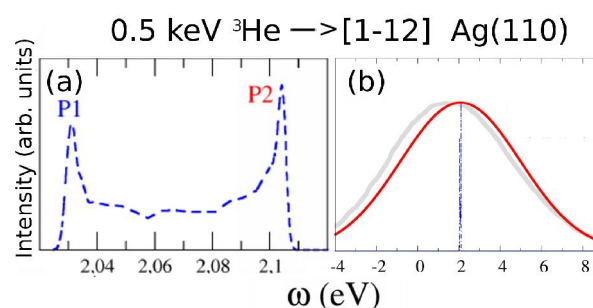


Figure 1. Energy-loss spectrum, as a function of the lost energy ω : (a) blue dashed line, results for a monoenergetic incident beam; (b) red solid line, results including the experimental energy spread; gray solid line, experimental data from Ref. [1].

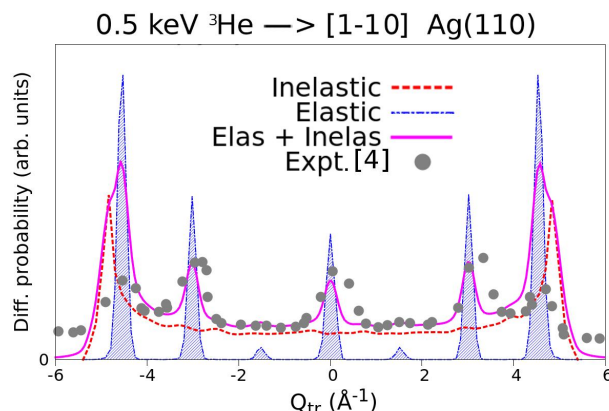


Figure 2. Momentum distribution, as a function of the transverse transferred momentum Q_{tr} , for the incidence angle $\theta_i = 0.75^\circ$.

References

- [1] Bundaleski *et al.* 2011 *NIMB* **269** 1216
- [2] J.I. Juaristi *et al.* 2008 *Phys. Rev. Lett.* **100** 116102
- [3] C. Ríos Rubiano *et al.* 2013 *Phys. Rev. A* **87** 012903; *idem.* 2014 *NIMB* **340** 15
- [4] Bundaleski *et al.* 2008 *Phys. Rev. Lett.* **101** 177601

E-mail: carior@iafe.uba.ar



Content from this work may be used under the terms of the [Creative Commons Attribution 3.0 licence](https://creativecommons.org/licenses/by/3.0/). Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.