The interaction of atoms with a LiF(001) surface revisited

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Synopsis Pairwise additive potentials for closed- and open- shell atoms interacting with a LiF(001) surface are revisited by including an improved description of the crystal electron density, as well as non-local electron density contributions. The electron distribution around each ionic site of the crystal is described with an *onion* model that takes into account the influence of the Madelung potential. From such densities, binary interatomic potentials are then derived by using well-known non-local functionals. Rumpling and contributions due to projectile polarization and van der Waals forces are also included. The potential model is assessed by contrasting angular positions of rainbow and supernumerary rainbow maxima produced by fast grazing incidence of He, N, Ne, S, Cl, Ar, and Kr with available experimental data.

In the field of particle-surface interactions, one of the most remarkable experimental advances of the past decade corresponds to the observation of grazing incidence fast atom diffraction (GIFAD or FAD), which has emerged as a powerful surface analysis technique. However, the accuracy of the surface information provided by the FAD method crucially relies on the theoretical model used to describe the surface potential.

In previous articles [1] the FAD process for a LiF surface was investigated by using a pairwise additive approach to represent the surface interaction. Pairwise additive potentials are built as a sum of binary interatomic potentials that describe the interaction of the atomic projectile with individual ionic centers of the crystal. For insulator materials, like LiF, this simple potential model has been shown to represent a reliable alternative to more complex self-consistent *ab initio* calculations. But in most works the binary potentials were derived by using the local density approximation (LDA), which does not include contributions due to non-local electron density terms.

In this work [2] we revisit previous pairwise additive models by incorporating non-local contributions of the electron density, together with the improvement of the description of the electron density associated with each ionic center of the insulator. Within this model, the interaction between rare gases (closed-shell atoms) (He, Ne, Ar, Kr, and Xe) with fully occupied valence shells, as well as open-shell atoms (N, S, and Cl) with vacancies in the outer level, and a LiF(001) surface is studied. In order to test the potential, we use it to evaluate angular distributions of fast atoms grazingly scattered from the surface along low-indexed crystallographic channels. The good agreement found for normal energies in the eV- range represents a meaningful evidence of the quality of the present model.

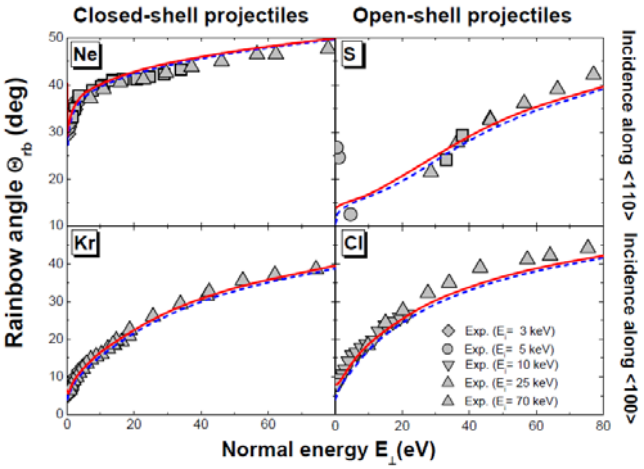

Figure 1. Rainbow deflection angle Θ_{rb}, as a function of the normal energy $E_\perp$. Red solid (blue dashed) line, results obtained including (neglecting) correlation [2].

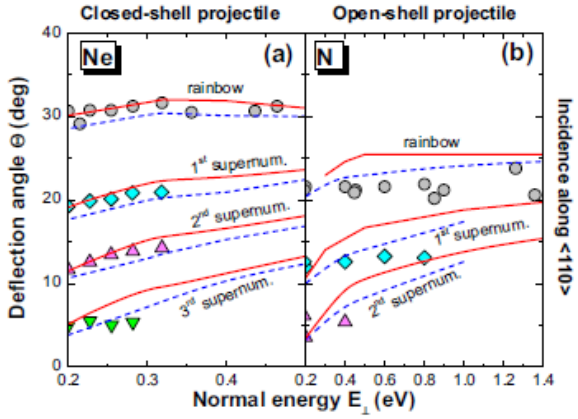

Figure 2. Deflection angles Θ corresponding to maxima of FAD distributions, as a function of the normal energy $E_\perp$. Lines, analogous to Fig. 1; symbols, experiment [2].

References

[1] M. S. Gravielle *et al* 2008 *Phys. Rev. A* 78 022901; ibid 2009 *Nucl. Instrum. Meth. Phys.Res* B 267 610; ibid. 2011 *Nucl. Instrum. Meth. Phys. Res. B* 269, 1208.

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