Dynamical Properties of an Atomic Interface Between fcc Lattices

Fazia Lekadir*, Rachid Tigrine

*Laboratory of Physics and Quantum Chemistry, M. Mammeri University, BP17 RP, 15000 Tizi Ouzou, Algeria,
Institute of Molecules and Materials du Mans UMR 6283, University du Maine, 72085 Le Mans, France
*Corresponding author: fazialekadir@yahoo.fr

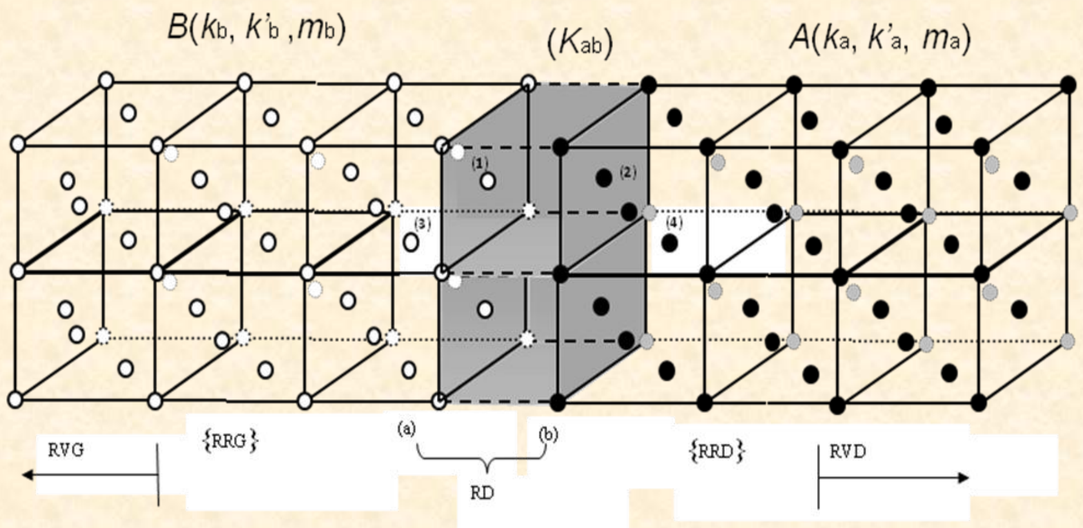
Abstract

A study of the phonon contribution to the interface properties between two fcc dissimilar solids is presented. The model system is obtained by the juxtaposition of two semi-infinite harmonic fcc lattices. The interface observables are numerically calculated for different cases of masses and elastic softening to hardening, to investigate how the local dynamics can respond to many environmental microscopic changes in the field interfacial domain. The theoretical formalism using simultaneously the Green's functions and the matching method is employed to describe the dynamics of the fcc system, the complete evanescent and the propagating fields. A calculation is presented for the vibration localized states, the coherent phonon transmission and the density of states (DOS), as element of a Landauer-Büttiker type scattering matrix.

The system dynamics, the phonon scattering and the transmission spectra via the interface domain between fcc lattices and the DOS are analyzed as function of the atomic masses and the elastic force constants occurring in the nanojunction zone of the model system.

Our results show that the interface zone is an effective phonon splitter and suggest that its characteristics may be controlled by varying its nanometric parameters. The observed fluctuations are due to the coherent coupling between continuum and discrete states induced by the interface domain.

System model



$$-\omega^2 m(l)u_\alpha(l,\omega)=\sum_{\lambda'}\sum_{\neq\lambda}\sum_{\beta}\left(\frac{r_\alpha r_\beta}{r^2}\right)K(l,l')\quad\left[u_\beta(l',\omega)-u_\beta(l,\omega)\right] \qquad (1)$$

❑ The systems established starting from the equation (1) can be written in the matrix form (2) following:

$$\left[\Omega^2 I - D\left(\vec{q},Z,Q_y,Q_z,r\right)\right]\left|u\right\rangle=0 \qquad (2)$$

❑ The Green functions are necessary to calculate the densities of states. In the matching method a very compact formulation of these functions, is obtained from the square matrix M_s under the operator form as (3):

$$G\left(\Omega^2+i\varepsilon,Q_y,Q_z,Z,r_i\right)=\left[\left(\Omega^2+i\varepsilon\right)I-M_s\left(Q_y,Q_z,Z,r\right)\right]^{-1} \qquad (3)$$

The spectral densities of the matrix, to a wave vector parallel to the direction of the magnetic interface are given by the following equation (4):

$$\rho_{(\alpha,\beta)}^{(p,p')}\left(\Omega,Q_y,Q_z\right)=2\Omega\sum_m L_{\alpha m}^{p}.L_{\beta m'}^{p'*}.\delta\left(\Omega^2-\Omega_m^2\right) \qquad (4)$$

Where p and p' represent two different spins, α and β two different Cartesian directions, and $L^p_{\alpha m}$ the component α of the vector amplitude of the vector spin precession p, for the energy branch Ω_m . The density of states which corresponds to the sum of Q_y, and Q_z trace matrices spectral densities can then be well written in the form (5):

$$D\left(\Omega\right)=\sum_{Q_y,Q_z}\sum_{p\alpha}\rho_{(\alpha,\beta)}^{(p,p')}\left(\Omega,Q_y,Q_z\right)$$

$$=-\frac{2\Omega}{\pi}\sum_{Q_y,Q_z}\sum_{p\alpha}\lim_{\varepsilon\to0^+}\left[\mathrm{Im}\,G_{\alpha\alpha}^{pp'}\left(Q_y,Q_z,\Omega^2+i\varepsilon\right)\right] \qquad (5)$$

Results

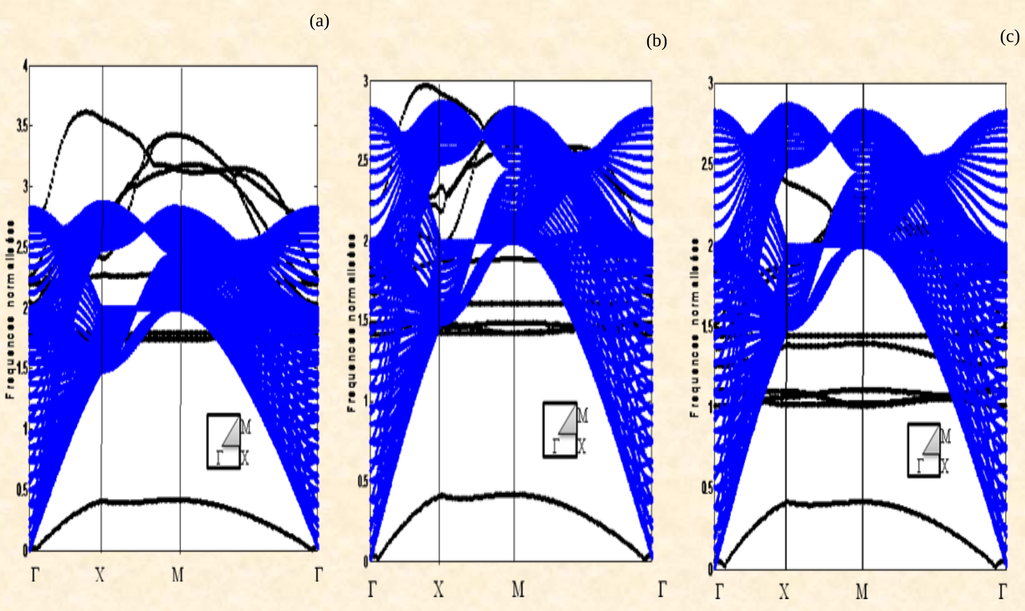


Fig.4 Calculated phonon dispersion curve presented in the principal directions of the Brillouin area. Interface states are indicated by the black curves. The blue lines represent the projection bulk phonon in the case of hardening in (a), homogeneity in (b) and softening in (c).

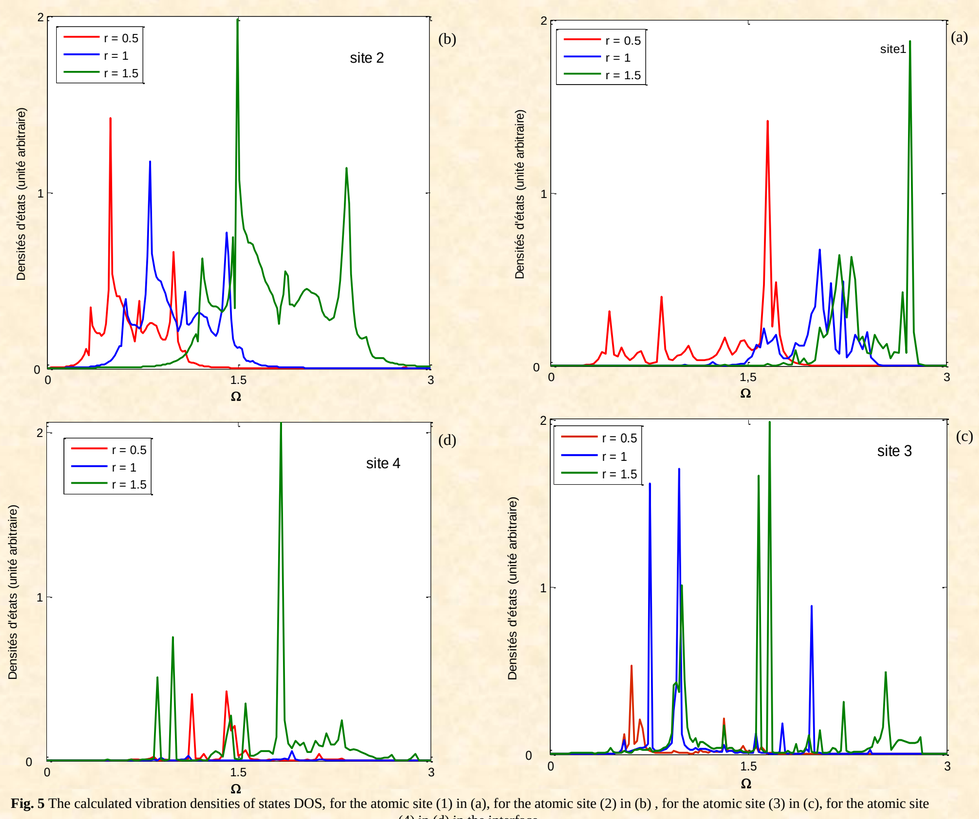


Fig. 5 The calculated vibration densities of states DOS, for the atomic site (1) in (a), for the atomic site (2) in (b) , for the atomic site (3) in (c), for the atomic site (4) in (d) in the interface.

Conclusions

In this work we investigate the vibrational properties of the bulk fcc cubic structure and the interface. We also calculate the localized phonons and associate state densities. The adapted matching method is used in this analytical and numerical study. Whereas we note that the ratio of constant forces strongly affects the curves of phonons localized. When the ratio force constant increases the phonon branches shift to high frequencies, and these branches are above the bulk band. When it decreases gradually the phonon branches are under the bulk band frequencies, and we also noted that the number of branches increases. We have shown the presence of three types of localized modes, the first mode is a Rayleigh , it spreads along the direction of high symmetry , the second type is the resonance located in the bulk band frequencies , the third is assigned to Einstein localized at high frequencies. Also we note the dependence of local densities of states, as the parameters of the system and the dimensionless frequencies..