GRAPHITE SURFACE PHONONS STUDIED THROUGH He ATOMS RESONANT SCATTERING

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Abstract.—He atom scattering has been used to study phonon-assisted bound state resonances and the Debye-Waller factor for the basal plane of graphite. A dispersion relation is reported for the surface phonons involved in the resonances. The attenuation of the specular peak in the temperature range from 20 to 315 K is used to derive the mean-square displacement $\langle u^2 \rangle$ of surface atoms, perpendicular to the (0001) plane. The anomalous thermal behaviour of $\langle u^2 \rangle$ is explained by considering the layered structure of the crystal.

Light atom scattering is in principle a powerful technique to study surface lattice dynamics. Detailed information on the dispersion relation of surface phonons can be obtained in special cases with the only study of angular distribution of the scattered particles, without any energy analysis. This is just what happens with the study of phonon assisted resonances, a process that was extensively studied recently for the He/graphite system [1].

We recall that the kinematic conditions for a scattering process involving the exchange of a single phonon are:

$$k^2 = k_0^2 + 2M\omega_q/\hbar$$  \hspace{1cm}  $$\vec{K}_G = \vec{K}_0 + \vec{G} + \vec{Q}$$  \hspace{1cm}  (1a-b)

where $\vec{k}$ is the wave vector of the gas atom of mass $M$, while $\hbar \omega_q$ and $\vec{Q}$ are the energy and parallel wave vector of the exchanged phonon; $\vec{G}$ is a surface reciprocal lattice vector. For in-plane scattering, a resonant structure in the angular distribution of the scattered atom, located at the polar angle $\theta^*_f$ and observed at incident angle $\theta^*_o$ must permit to obtain $\hbar \omega^*_q$ and $\vec{Q}^*$ for the involved phonon through the solution of the two equations:

$$k_0^2 + 2M\omega^*_q/\hbar - (\vec{K}_0 + \vec{Q})^2 - 2M \varepsilon_j/\hbar^2 = 0$$  \hspace{1cm}  (2)
where Eq. 2 represents the condition for an atom to enter a bound state $(E_j, N)$ while Eq. 3 is the condition for the atom to be scattered at a given final angle $\theta_f$ through the final $F$ diffraction channel. The resonant state labeled $(E_j, N)$ is an intermediate state in which the atom is diffracted in a closed channel $N$, with its perpendicular energy negative and equal to an energy level $E_j$ of the atom-surface potential $\kappa^2k_N^2/2M = E_j < 0$.

For He/graphite system we selected and analysed about 120 angular distributions, where about 180 resonance structures were identified. Details of the experiment are reported elsewhere $[1,2]$. The angular positions of the resonant structures $(\theta_o, \theta^*_f)$ gave, through Eqs. 2 and 3 the $\kappa\omega_q^*$ and $\theta^*$ of the phonon involved in the resonance. All the observed points belong to a limited region of the surface projected phonon dispersion relation $\omega(Q)$. The best fit region of the experimental points is reported in Fig. 1 as a dashed area, and compared with the dispersion relations $\omega(Q)$ for bulk phonons travelling along the $\Gamma M$ direction, as obtained by neutron scattering $[3]$. The experimental region contains the transverse acoustic mode $TA_1$ for bulk phonons; this seem to indicate a strong contribution of Rayleigh phonons to surface scattering.

In order to study the thermal vibration at the surface, the specularly reflected intensity was also measured at several incident angles, for surface temperatures $20 K < T_S < 315 K$. The thermal attenuation of the specular beam was represented by the conventional Debye-Waller formula $P_{el} = P_{exp} \exp(-2\lambda)$, where the D-W coefficient for atom scattered by surfaces is $2\lambda = q_z^2 \langle u_1^2 \rangle$, $q_z$ being the momentum transfer perpendicular to the surface. The elastic probability $P_{el}$ was calculated in the eikonal approximation and the $\langle u_1^2 \rangle$ values were obtained from $P_{exp}$. The average values obtained at different surface temperatures are reported in Fig. 2 with their statistical error. The $\langle u_1^2 \rangle$ value at room temperature is in agreement with the bulk value obtained by Chen and Trucano $[4]$, who evaluated a Debye temperature of about 530 K. However the temperature dependence does not follow the Debye curve, reported in Fig. 2 (curve (a)). We tried to explain the appreciable
Fig. 1: Most probable experimental dispersion relation of surface phonon (dashed region) compared with the bulk phonon spectrum in the ΓM direction (Ref. 3).

The decrease of $\langle u^2 \rangle$ at low temperature taking into account of the anisotropy and the layered structure of graphite crystal. We assumed a quadratic dispersion relation at low $Q$, as obtained by neutron data [3] and by atom scattering. Details of this calculation are reported elsewhere [2]. The $\langle u^2 \rangle$ so calculated is reported in Fig. 2 (curve (b)). It appears that the temperature dependence of the experimental points is now well reproduced. The remaining shift of curve (b) can be attributed to both some uncertainty in the absolute experimental intensities and to the simplified assumed phonon spectrum.

References