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APPLICATION OF SURFACE WAVES FOR STUDYING THE CHARACTERISTICS OF GAS-TRAPPING SENSORS LOCATED ON A SOLID SURFACE

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Dispersion relations for surface waves and attenuation parameters in a crystal with the impurity monolayer adsorbed on its top are studied. We consider a face-centered cubic crystal with central interaction between the nearest neighbors as a model and calculate the value of m_0^* for the adsorbed surface monolayer. Beginning from it ($m_0 < m_0^*$), the surface wave splits off the upper edge of the volume spectrum and attenuates non-monotonously (with oscillations), when penetrating into the crystal bulk.

K e y w o r d s: volume and surface waves, dispersion relations, amplitude decreasing parameter, adsorbed surface monolayer.

1. Introduction

Current trends in engineering allow one to build up the atomic (nanoscale) architecture of the surface of solid supports in a controlled manner [1]. The microfabricated surfaces of acoustic-wave sensors can be made highly responsive to the mass adsorbed from a gas, vapor, or liquid phase [2]. In particular, the devices with surface acoustic waves are widely used for the precise gravimetrical measurements of negligible masses by chemical sensors and biosensors [2, 3]. In this context, the theoretical analysis and the modeling of the dynamics of a propagation of acoustic waves in the adsorbed monolayer on the surface of an oscillating crystal is an important part of the research of sensors [4–6].

In the present work, we consider the surface vibrations of pure shear waves in the case of the (001) surface orientation in face-centered cubic crystals with adsorbed surface monolayer. The characteristics of surface waves are highly sensitive to properties of the surface. In this connection, the pure shear surface waves with horizontal polarization (SH-waves) are of great interest both in the context of fundamental studies and technological applications [5, 7, 8].

Consider the elastic vibrations of an FCC crystal with interaction between the nearest neighbors taken into account. We describe our system in a scalar model, i.e. the displacement of an atom from its equilibrium state is described with the scalar value $u(\mathbf{n})$, ($\mathbf{n}(n_1, n_2, n_3)$ is an integer-valued vector enumerating the lattice points). The equation of motion of such a system in the harmonic approximation is given by [5].

$$m\,(\mathbf{n})\,\frac{\partial^2 u(n)}{\partial t^2} = -\sum_{n'} \alpha(\mathbf{n}, \mathbf{n}')u(\mathbf{n}'). \qquad (1)$$

Here, $m(\mathbf{n})$ is the atomic mass at the n^{th} node; $\alpha(\mathbf{n},\mathbf{n}')$ are force coefficients. Let the crystal be bounded with (001) surface, and let the outer atomic layer ($n_3 = 0$) consist of impurity atoms (m_0 is the mass of an impurity atom, and m is the mass of a host one; see Fig. 1). The force constants for the nearest neighbors are

$$\alpha(\mathbf{n},\mathbf{n}') = \begin{cases} \alpha; & n_3, n_3' \geq 1; \quad \text{(a)} \\ \gamma\alpha; & n_3 = 0,\ n_3' = 1; \quad \text{(b)} \\ \gamma'\alpha; & n_3, n_3' = 0. \quad \text{(c)} \end{cases} \tag{2}$$

In Eq. (2), we allow for the interaction $\gamma\alpha$ between the surface ($n = 0$) and subsurface ($n = 1$) layers to be different from the interlayer interaction α in the bulk. In addition, expression (2c) allows one to take a surface distortion into account.

The occurrence of the translational invariance along (001) plane allows one to find the eigenvibrations as $u(n_1, n_2, n_3) = u(n_3)\exp[i(k_1 n_1 + k_2 n_2) - -i\omega t]$, where k_1 and k_2 are components of the dimensionless plane wave vector $\chi(k_1, k_2)$, and ω is the oscillation frequency. Since there is the translation invariance in the (xy) plane (z axis is perpendicular to the plane), k_1 and k_2 are "good" quantum numbers, and we will seek the frequency dependence on $\chi(k_1, k_2)$. k_3 runs all values from 0 to π. Denoting $u(n_3) \equiv u(n)$, we obtain the following expressions from Eq. (1):

$$\frac{m_0\omega^2 u(0)}{\alpha} = 4(\gamma + \gamma')u(0) - \\ - 4\gamma(\cos k_1 + \cos k_2)wu(1); \quad (n = 0); \tag{3}$$

$$\frac{m\omega^2 u(1)}{\alpha} = (8 + 4\gamma)u(1) - 4u(1)\cos k_1 \cos k_2 - \\ - 2(\cos k_1 + \cos k_2)(u(2) + \gamma u(0)); \quad (n = 1); \tag{4}$$

$$\frac{m\omega^2 u(2)}{\alpha} = 12u(2) - 4u(1)\cos k_1 \cos k_2 - \\ - 2(\cos k_1 + \cos k_2)(u(2) + \gamma u(0)); \quad (n = 2). \tag{5}$$

For $n \geq 2$, relation (5) is a system of linear homogeneous finite difference equations of the second order with constant coefficients. The sequence $\{u(n)\}$, $n = 1, 2, ...$, determined by the system is actually a sum of geometric progressions

$$u(n) = \sum_{j=2}^{2s} V_j q_j^n, \quad |q| < 1, \tag{6}$$

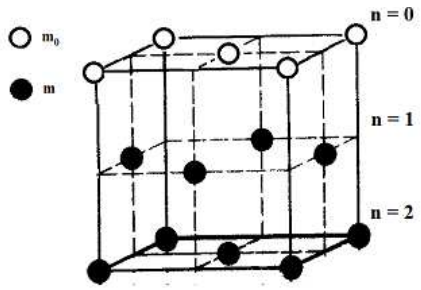

Fig. 1. Semi-infinite face-centered cubic crystal with an adsorbed impurity monolayer on its top

V_j are the amplitudes of $2s$ partial waves characterized by q_j parameters depending on the wave vector χ and the wave frequency ω and determine the attenuation of a given partial wave into the crystal bulk; i.e. q determines the penetration depth. Hereafter, we are going to consider the single-partial surface waves, for which $u(n) = u(1)q^{n-1}$ in the considered model, and Eq. (5) for a layer with $n \geq 2$ can be rewritten as

$$\frac{m{\omega_s}^2}{\alpha} = (12 - 4\cos k_1 \cos k_2) - \\ - 2(\cos k_1 + \cos k_2)\left(q + \frac{1}{q}\right), \tag{7}$$

and $u(0)$ is a an independent component (the surface impurity mass m_0 differs from the host mass m) and comes out of the geometric progression.

Relations (3) and (4) are boundary conditions.

Let us consider an FCC crystal without surface distortion ($\gamma = \gamma' = 1$). The dispersion relation for volume vibrations is

$$\frac{m}{\omega_V^2}\alpha = 12 - 4\cos\left[k_1\frac{a_0}{\sqrt{2}}\right]\cos\left[k_2\frac{a_0}{\sqrt{2}}\right] - \\ - 4\cos\left[k_1\frac{a_0}{\sqrt{2}}\right]\cos\left[k_3\frac{a_0}{\sqrt{2}}\right] - \\ - 4\cos\left[k_2\frac{a_0}{\sqrt{2}}\right]\cos\left[k_3\frac{a_0}{\sqrt{2}}\right]. \tag{8}$$

The borders of the two-dimensional Brillouin zone along the symmetric directions are shown in Fig. 2. Without any loss of generality, we choose the $k = k_1 = k_2$ direction of the two-dimensional Brillouin zone.

In this case, expression (7) transforms into

$$\frac{m{\omega_s}^2}{\alpha} = (12 - B) - A\left[q + \frac{1}{q}\right], \tag{9}$$

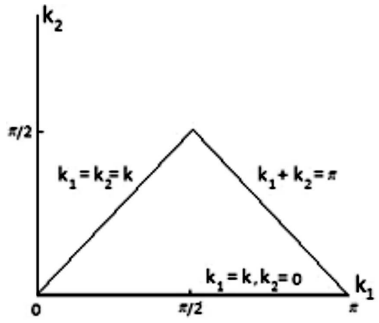

Fig. 2. Two-dimensional Brillouin zone for an FCC crystal

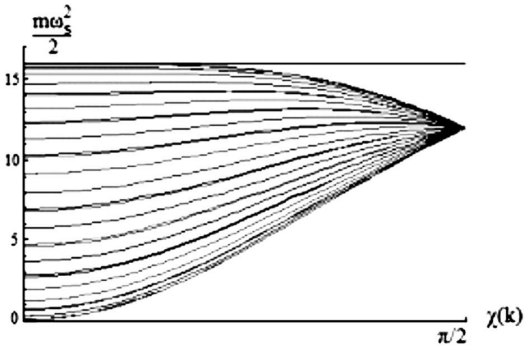

Fig. 3. Volume vibration band and surface waves in a face-centered cubic crystal with adsorbed surface monolayer; $m_0/m = 0.5$

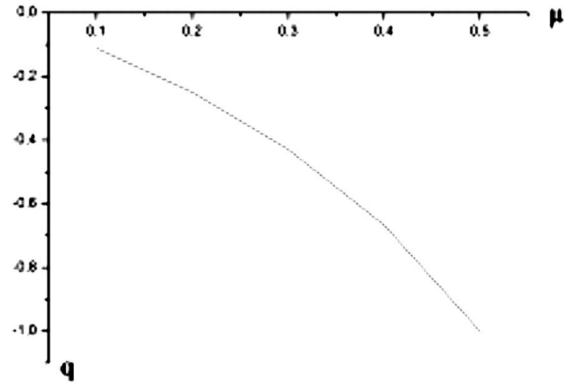

Fig. 4. Dependence of the decreasing parameter q on the impurity mass

where

$$A = 2\left(\cos\left[k_1\frac{a_0}{\sqrt{2}}\right] + \cos\left[k_2\frac{a_0}{\sqrt{2}}\right]\right);$$
$$B = 4\cos\left[k_1\frac{a_0}{\sqrt{2}}\right]\cos\left[k_2\frac{a_0}{\sqrt{2}}\right]. \tag{10}$$

The equations for the defect ($n = 0$) and intermediate ($n = 1$) layers are

$$\begin{cases} \dfrac{m_0\omega_s^2}{\alpha}u(0) = (8-B)\,u(0) - A\,u(1), \\ \dfrac{m{\omega_s}^2}{\alpha}u\,(1) = (12-B)\,u\,(1) - A\,[u\,(1)\,q + u\,(0)]. \end{cases} \tag{11}$$

From (4) and (6), we obtain the expressions for the dispersion relation of surface waves and the decreasing parameter q depending on $\mu = m_0/m$. Consider the case of light impurity atoms, $\mu = m_0/m < 1$. Thus, we obtain

$$q = \frac{8 - B - (12-B)\,\mu}{2A(1-\mu)} - \\ - \frac{\sqrt{4A^2(\mu-1)\mu + (B - 8 + (12-B)\mu)^2}}{2A(1-\mu)}. \tag{12}$$

The dispersion relation is calculated from (9).

Let us analyze the obtained expression for some particular value $\mu = 0.1$ (the adsorbed atom is ten times lighter than the host one). Then

$$q = -\frac{B - 8 + 0.1(12-B)}{1.8A} + \\ + \frac{\sqrt{-0.36A^2 + (8 - B + 0.1(B-12))^2}}{1.8A}. \tag{13}$$

Here, $q < 0$, $|q| < 1$, i.e. the oscillation amplitude decreases non-monotonously (with oscillations), while penetrating into the crystal bulk.

It is easy to calculate the splitting of the surface wave from the volume band. We have

$$\Delta = \frac{m{\omega_s}^2}{\alpha} - \frac{m{\omega_{v\max}}^2}{\alpha} = A\left(q + \frac{1}{q}\right). \tag{14}$$

It is greater than zero, if $\mu \le 0.5$, i.e. the surface waves split off higher than the highest edge of the volume band. For $\mu = 1/2$, the dispersion relation for surface waves does not depend on the wave vector $\chi\,(k_1, k_2) = \chi\,(k)$,

$$\frac{m{\omega_s}^2}{\alpha} = 16, \tag{15}$$

and is a straight line on the $\omega^2(\chi)$ dependence (Fig. 3).

Moreover, the essential condition $|q| < 1$ is fulfilled only if $\mu \le 0.5$ (Fig. 4).

For $ka \ll 1$, the splitting parameter $\triangle$ takes very small values, and the surface wave penetrates deeply

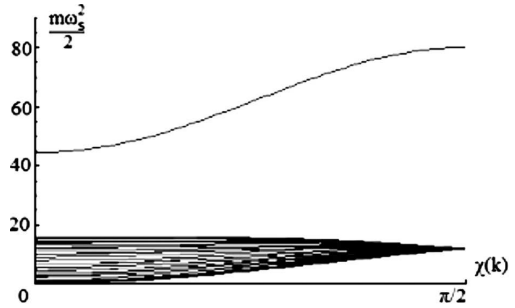

Fig. 5. Volume vibration band and surface waves in a face-centred cubic crystal with adsorbed surface monolayer; $m_0/m = 0.1$

into the crystal bulk (quasivolume). But, in the short-wave approximation, the penetration depth of a surface wave decreases, as $\chi(k)$ increases. For $k = \frac{\pi}{2}$, the surface wave is localized only in the impurity surface monolayer.

Since the frequency is dependent on the m_0/m ratio, it is possible to determine the impurity mass with the dispersion relation obtained or by the spreading the velocity of the surface wave $\frac{\partial\omega}{\partial k}$. The dependence of ${m\omega_s}^2/\alpha$ on the two-dimensional vector $\chi(k_1, k_2) = \chi(k) = \left[0; \frac{\pi}{2}\right]$ is shown in Fig. 5.

Since $q < 0$, the surface wave oscillations decrease non-monotonously in the case of light impurity atoms, while penetrating into the crystal bulk. The surface vibrations are high-frequency presented as a single curve splitting off the highest edge of the continuous spectrum of volume vibrations.

Therefore, the impurity mass, at which a surface wave splits exactly off the top of the continuous spectrum has been calculated, and it is five times lighter than the mass of a host atom. For $\mu \leq 0.5$, the surface wave splits off higher than the highest edge of the volume vibration band. For $\mu > 0.5$, the inequality $|q| < 1$ is not fulfilled. So, the high frequency surface waves are not excited at such ratios. The vibrations of light impurity atoms in the surface monolayer are high-frequency; their amplitudes decrease non-monotonously, as the surface wave penetrates into the crystal bulk. In the long-wave approximation ($ka \ll 1$), the vibrations penetrate deeply, being quasivolume, while they are localized only in the impurity monolayer for $k = \pi/2$ (short-wave approximation).

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ЗАСТОСУВАННЯ ПОВЕРХНЕВИХ ХВИЛЬ ДЛЯ ВИВЧЕННЯ ХАРАКТЕРИСТИК ГАЗОЧУТЛИВИХ СЕНСОРІВ НА ПОВЕРХНІ ТВЕРДОГО ТІЛА

Р е з ю м е

В роботі отримано закони дисперсії та параметри загасання поверхневої хвилі у кристалі з домішковим моношаром, адсорбованим на поверхні. У ролі моделі розглянуто гранецентровану кубічну ґратку із центральною взаємодією між найближчими сусідами. Обчислено значення домішкової маси m_0^*, починаючи з якої ($m_0 < m_0^*$) поверхнева хвиля відщеплюється від верхньої границі спектра об'ємних коливань та затухає немонотонно (з осциляціями) із поширенням в глибину кристала.