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2008 J. Phys.: Condens. Matter 20 224025

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Local vibrational states in real crystals with impurities near the surface

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Received 8 November 2007

Published 13 May 2008

Online at stacks.iop.org/JPhysCM/20/224025

Abstract

Local vibrational states (LVS) induced by a combined defect ‘impurity–sample surface’ are discussed. An analytical approximation for the basic characteristics of the LVS is derived. The approach developed can serve as an useful tool for the analysis of measured local frequencies and intensities of LVS, and can also be employed to gain information on the interatomic interactions and defect structure.

1. Introduction

As it is known, lightly or strongly-coupled impurities can generate LVS (namely discrete vibrational levels in a crystal that are located beyond the band of the quasi-continuous phonon spectrum of a perfect lattice). The amplitudes of the local vibrations decrease rapidly on moving away from the defect. When the distance from the impurity atom becomes much larger than the characteristic radius of the interatomic interaction in the lattice, the amplitudes vanish exponentially.

For over six decades LVS have been investigated both theoretically (see e.g., [1–10]) and experimentally [5, 6, 11–17]. The results obtained in this area can be found in monographs on crystal lattice dynamics, for example in [18–22]. Numerical simulations [4–6] have led to significant progress in studying the formation conditions and characteristics of LVS, such as the frequencies.

Measured local vibration characteristics can be used to deduce valuable information on the defect structure and force interactions in real crystals. The quantities usually obtained in experiments are the frequencies of the local vibrations. For the analysis of experimental data it is essential to have analytical expressions that relate the basic characteristics of LVS to the parameters of the defect and the host lattice.

In this paper, LVS caused by the presence of a combined ‘impurity–sample surface’ defect are studied with the approach developed in [7] for constructing analytical approximations for the formation conditions and the characteristics of LVS. The analysis carried out can be of interest in interpreting data obtained via the methods of optical and point–contact

spectroscopy, both very powerful techniques for experimental investigation of LVS.

2. Analytical description of local vibration characteristics

The analytical approximation [7] proved to be a convenient method providing a high-accuracy description of local vibration frequencies in the phonon spectra of impurity-containing crystals. The procedure is based on the vibration classification accepted in the *Jacobian-matrix* (\mathcal{J} -matrix) method [23–25] and is essentially different from the traditional plane–wave expansion.

In the \mathcal{J} -matrix approach the space H of atomic displacements in an arbitrary system is divided into subspaces $H^{(i)}$ that are invariant with respect to the $\hat{\mathcal{L}}$ -operator describing the crystal lattice vibrations. Each of the subspaces $H^{(i)}$ is a set of all linear combinations of the vectors in the sequence

$$\left\{ \hat{\mathcal{L}}^n \vec{h}_0^{(i)} \right\}_{n=0}^{\infty} = \vec{h}_0^{(i)}, \hat{\mathcal{L}} \vec{h}_0^{(i)}, \hat{\mathcal{L}}^2 \vec{h}_0^{(i)}, \dots, \hat{\mathcal{L}}^n \vec{h}_0^{(i)}, \dots \quad (1)$$

Here $\vec{h}_0^{(i)}$ is vector which belongs to the space of the atomic displacements H with the operator $\hat{\mathcal{L}}$. In the basis $\{\vec{h}_n^{(i)}\}_{n=0}^{\infty}$ obtained by orthonormalization of the sequence (1) the operator $\hat{\mathcal{L}}^{(i)}$ induced by the operator $\hat{\mathcal{L}}$ in the subspace $H^{(i)}$ can be written as a tridiagonal \mathcal{J} -matrix $\hat{\mathcal{L}} = \mathcal{L}_{ik} = a_n \delta_{ik} + b_n (\delta_{i,k+1} + \delta_{i+1,k})$ having a simple spectrum (hereinafter the index (i) indicating subspaces is omitted). The local Green function (LGF) $\mathcal{G}(\lambda)$ of the system is the matrix element $\mathcal{G}_{00}(\lambda)$ of the operator $\hat{\mathcal{G}}(\lambda) = (\lambda \hat{\mathcal{T}} - \hat{\mathcal{L}})^{-1}$, where $\hat{\mathcal{T}}$ is the unit

operator, $\lambda \equiv \omega^2$ is the $\hat{\mathcal{L}}$ -operator eigenvalue. The LGF can be written as [23–25]

$$\mathcal{G}(\lambda) = \lim_{n \rightarrow \infty} \mathcal{G}_{(n)}(\lambda);$$

$$\mathcal{G}_{(n)}(\lambda) = \frac{\mathcal{Q}_n(\lambda) - b_{n-1} \mathcal{Q}_{n-1}(\lambda) \mathcal{K}_\infty(\lambda)}{\mathcal{P}_n(\lambda) - b_{n-1} \mathcal{P}_{n-1}(\lambda) \mathcal{K}_\infty(\lambda)} \quad (2)$$

where $\mathcal{P}_n(\lambda)$ and $\mathcal{Q}_n(\lambda)$ are the polynomials of degree n and $n - 1$, respectively. If the quasi-continuous spectrum band is simply connected, i.e. $\omega \in [0; \omega_m]$, the following limiting-value equations are valid for the matrix elements a_n and b_n : $\lim_{n \rightarrow \infty} a_n = 2 \lim_{n \rightarrow \infty} b_n = \lambda_m/2$. The function

$$\mathcal{K}_\infty(\lambda) = 4\lambda_m^{-2} \{2\lambda - \lambda_m + 2\mathcal{Z}(\lambda) \sqrt{\lambda |\lambda - \lambda_m|}\},$$

where $\mathcal{Z}(\lambda) \equiv i\Theta(\lambda) \Theta(\lambda_m - \lambda) - \Theta(\lambda - \lambda_m)$ and $\Theta(x)$ is the Heaviside function, is obtained by contracting a continued fraction corresponding to the \mathcal{J} -matrix whose elements are equal to their asymptotic values.

From equation (2) one can conclude that spectral density of states

$$\rho(\lambda) = \pi^{-1} \text{Im} \mathcal{G}(\lambda) \quad (3)$$

is the so-called ‘regular’ or ‘elliptic’ squared-frequency distribution (see, e.g. [21]) modulated by a certain $2n$ -power polynomial. The spectral density (3) is commonly used in approximate calculation and is normalized per unit. Both the function $\rho(\lambda)$ and the approximation of the real part of the Green function given by equation (2) are analytical inside the continuous spectrum band. This approximation of the real and imaginary parts of the Green function is not exact in the continuous spectrum band, where $\text{Re} \mathcal{G}(\lambda)$ and $\text{Im} \mathcal{G}(\lambda)$ are not analytical functions. The local Green function is an analytical function beyond the continuous spectrum band. As is demonstrated in [7] and as is discussed in the next section of this paper, the convergence rate of this function is very high as n increases and the approximations of equation (2) for $n = 1$ and for $n \gg 1$ coincide to a high degree of accuracy.

One can expect that the use of LGF $\mathcal{G}_{(1)}(\lambda)$ will yield a satisfactory description of LVS. Derivation of analytical expressions for the first matrix elements a_0 and b_0 of the \mathcal{J} -matrix and, hence, for the function $\mathcal{G}_{(1)}(\lambda)$ can be accomplished straightforwardly.

The frequencies of LVS are solutions of the Lifshitz equation [2], which can be written in the form

$$\mathcal{S}(\lambda) = \mathcal{S}(\lambda, \hat{\Lambda}), \quad \lambda > \lambda_m. \quad (4)$$

The function $\mathcal{S}(\lambda, \hat{\Lambda})$ describes the influence of the defect and depends on the corresponding parameters of the perturbation operator $\hat{\Lambda}$. In the case of a degenerate regular perturbation [2], one can obtain an exact expression for this function. Thus for a substitutional isotopic impurity one has

$$\mathcal{S}(\lambda, \hat{\Lambda}) \equiv \mathcal{S}(\lambda, \varepsilon) = -1/(\omega^2 \varepsilon), \quad (5)$$

where $\varepsilon \equiv (\tilde{m} - m)/m$ is the mass defect of the impurity, \tilde{m} is the mass of the impurity, and m is the mass of an atom of the host lattice.

In many cases direct determination of the poles of the Green function

$$\tilde{\mathcal{G}}(\lambda) \equiv \left(\vec{h}_0, \left[\lambda \hat{\mathcal{X}} - \hat{\mathcal{L}}_0 - \hat{\Lambda} \right]^{-1} \vec{h}_0 \right)$$

of a perturbed system, that corresponds to the use of the \mathcal{J} -matrix of the operator $\hat{\mathcal{L}} = \hat{\mathcal{L}}_0 + \hat{\Lambda}$ in equation (2), can be a constructive alternative to treatment of the Lifshitz equation. This procedure can also be employed for finding the LVS caused by a non-degenerated perturbation operator, when the perturbation does not affect the width of the continuous spectrum band, or, in other words, when the perturbation leaves the limiting values of the \mathcal{J} -matrix intact. Such a perturbation can be considered as ‘asymptotically degenerate’. The poles of the Green function λ_d are the frequencies of local vibrations squared. The residues of λ_d at the poles $\mu_0^{(d)} \equiv \text{rés}_{\lambda=\lambda_d} \mathcal{G}_{00}(\lambda)$ determine the intensities, thus characterizing the amplitude of the same discrete-frequency vibrations in the subspace induced by the vector \vec{h}_0 .

One can introduce the parameters η and ζ , describing the deviation of the matrix elements a_0 and b_0 from their limiting values

$$a_0 = a/(1 + \eta), \quad b_0 = b/\sqrt{1 + \zeta},$$

$$\eta, \zeta \in [-1, +\infty), \quad (6)$$

and get for the squared LVS frequency [7]

$$\lambda_1(\eta, \zeta) \equiv \omega_1^2(\eta, \zeta) = \frac{\lambda_m}{4\zeta(1 + \eta)}$$

$$\times \left\{ 2\zeta - \eta - \sqrt{-\zeta + \frac{(\eta - \zeta)^2}{1 + \zeta}} \right\}. \quad (7)$$

The local vibration exists when

$$\zeta < -3/4; \quad \eta \in [-1, +\infty); \quad \text{or}$$

$$\zeta > -3/4; \quad \eta < -(1 + 2\zeta)/(3 + 4\zeta). \quad (8)$$

If equation (8) is satisfied and the local vibrational state exists, its intensity is given by

$$\mu_0 = \left(\eta + (1 + 2\zeta) \sqrt{-\zeta + \frac{(\eta - \zeta)^2}{1 + \zeta}} \right)$$

$$\times \left(2\zeta \sqrt{-\zeta + \frac{(\eta - \zeta)^2}{1 + \zeta}} \right)^{-1}. \quad (9)$$

Substitution of (7) into the Lifshitz equation shows that $\lambda_1(\eta, \zeta)$ obeys this equation when (8) is satisfied.

The attenuation of the vibrations can be characterized by a decrease of their amplitudes with the growth of the ‘number’ n . As demonstrated in [7], the variations of the amplitudes are proportional to $\mathcal{P}_n^2(\lambda_1)$. The values of μ_n form a geometric progression $\mu_n = \mu_1 q^{n-1} = \frac{\mu_0}{1 + \zeta} q^n$ for $n \geq 1$ if they are non-zero, i.e. when the requirement of equation (8) is satisfied

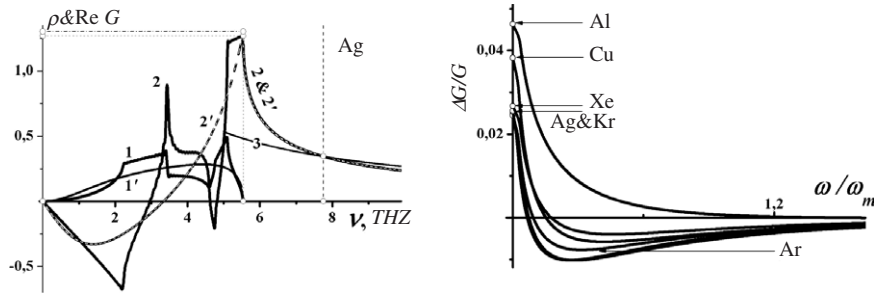


Figure 1. Approximation for the Green function $\mathcal{G}_{(1)}(\omega)$ and $\mathcal{G}_{(76)}(\omega)$ of Ag and the solution of Lifshitz equation (left). Relative deviation of this approximation for various fcc crystals (right).

and the local levels really exist. The denominator of this progression $q = [\sqrt{1 + \zeta} \mathcal{P}_1(\lambda_1)]^2$ can be written as

$$q = \left\{ \frac{(1 + \zeta)}{\zeta(1 + \eta)} \left[\eta + \sqrt{-\zeta + \frac{(\eta - \zeta)^2}{1 + \zeta}} \right] \right\}^2.$$

The quantity q is less than unity under the condition of equation (8); at the same time $\sum_{n=0}^{\infty} \mu_n = 1$.

Having found the functions η and ζ for particular crystalline structures with various defect configurations and substituting them into equations (7)–(9), we can obtain the dependencies of the formation conditions and the dynamic characteristics of LVS on the parameters describing defects and a perfect lattice.

3. Local vibrations caused by near-surface substitutional impurity

Let us consider the fcc crystal lattices of some metals (Ag, Cu, Al) and solid rare gases (Ar, Kr, Xe). The description of the interatomic interaction in these substances can be reduced to the interaction between the nearest neighbors [21, 27]. The matrices of force constants are [28]

$$\Phi_{ik} \left(\mathbf{r}, \mathbf{r} + \left[\frac{a}{2}; \frac{a}{2}; 0 \right] \right) = - \begin{pmatrix} \alpha & \gamma & 0 \\ \gamma & \alpha & 0 \\ 0 & 0 & \beta \end{pmatrix}. \quad (10)$$

The force constant matrices for the rest of the nearest neighbors $\mathbf{r} + \Delta$ can be found from equation (10) using O_h -point group symmetry operations. The translation invariance condition results in the self-action matrix $\Phi_{ik}(\mathbf{r}, \mathbf{r}) = - \sum_{\Delta} \Phi_{ik}(\mathbf{r}, \mathbf{r} + \Delta)$, which has the form $\Phi_{ik}(\mathbf{r}, \mathbf{r}) = 4(2\alpha + \beta)\delta_{ik}$.

The left-hand side of figure 1 shows the dependencies of the spectral density $\nu(\omega) = \pi^{-1} \text{Im} \mathcal{G}(\omega)$ (curves 1 and 1') and the real part of the Green function $\mathcal{G}_{(n)}(\omega) \equiv 2\omega \mathcal{G}_{(n)}(\lambda)$ (curves 2 and 2') on the frequency ω . The force constants α , β , and γ were obtained in [26]. Curves 1 and 2 correspond to $n = 76$, the dashed lines 1' and 2' are for $n = 1$. As can be seen, in the continuous spectrum band $\omega \in [0, \omega_m]$ the results of the calculations for $n = 1$ and for $n = 76$ differ significantly, while outside this band at $\omega > \omega_m$ curves 2 and 2' are very close to each other, except for the very narrow region near the maximum frequency ω_m of the continuous spectrum.

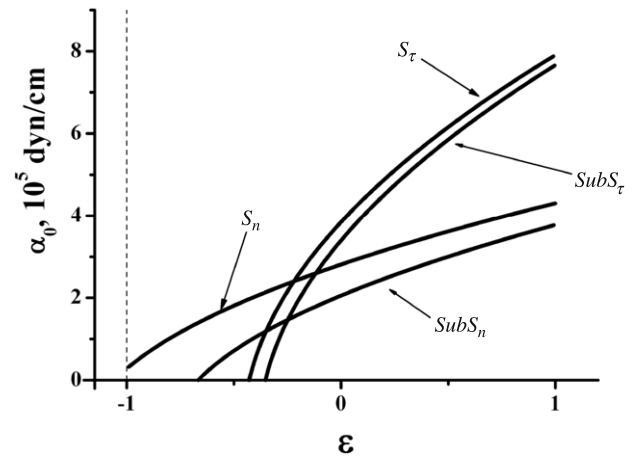


Figure 2. Regions where LVS exist for displacements of a surface atom along the normal to the surface S_n and along the surface S_τ , as well as for displacements of a subsurface atom $SubS_n$ and $SubS_\tau$. LVS appear in the areas above the corresponding curves.

The right-hand side of figure 1 shows the relative deviation of the approximation $\mathcal{G}_{(1)}(\omega)$ from $\mathcal{G}_{(76)}(\omega)$

$$\Delta \equiv (\mathcal{G}_{(1)}(\omega) - \mathcal{G}_{(76)}(\omega)) / \mathcal{G}_{(76)}(\omega) \quad (11)$$

as a function of the frequency in the region $\omega \geq \omega_m$ for the perfect crystal lattices of Ag, Cu, Al, Ar, Kr, and Xe. One can see that the values of Δ vary from $\sim 1\%$ near ω_m to ~ 0.1 – 0.01% at an appreciable distance from the edge of the continuous spectrum.

As an example, the left-hand side of figure 1 illustrates the graphical solution of the Lifshitz equation [2, 23] for the case of an isolated Al impurity. The Al admixture to Ag behaves as a light isotopic substitutional impurity [21]. Curve 3 in this figure corresponds to the function $\mathcal{S}(\omega, \varepsilon) = -2/(\omega \varepsilon)$ [10, 23] with $\varepsilon \approx -0.74987$. The ω -values at which this curve crosses the $\mathcal{G}_{(76)}(\omega)$ and $\mathcal{G}_{(1)}(\omega)$ curves, being the local frequencies, coincide within $\sim 10^{-4}$. In the isotopic approximation adopted by us, the Al impurity in Ag generates LVS with frequency $\nu_l \approx 7.752$ THz.

For an impurity, that is not isotopic in the bulk, the force constants of the interaction can be found from

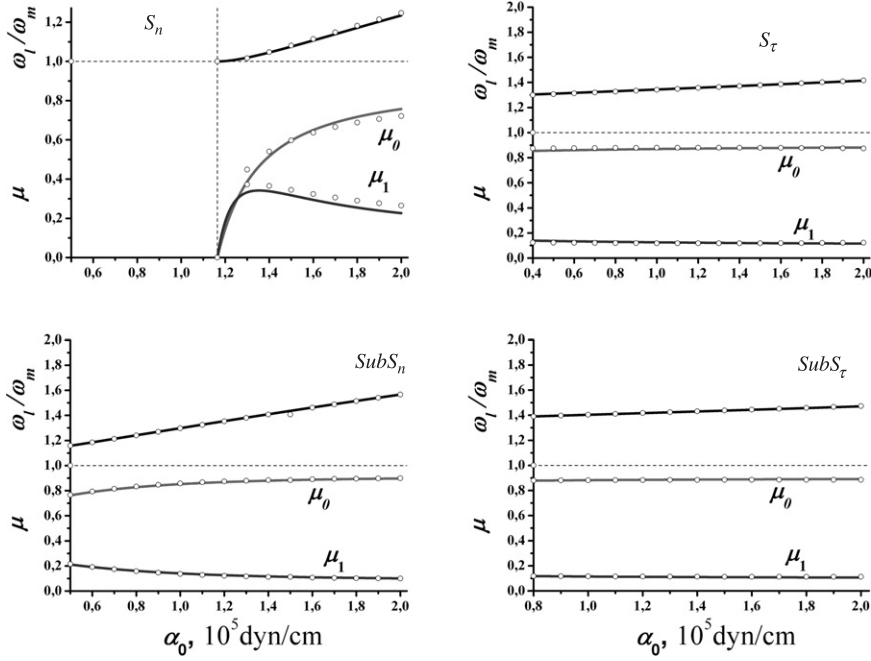


Figure 3. Dependence of the frequencies and intensities of LVS on the parameter α_0 .

equations (6), (7) and (9) with

$$\eta(\varepsilon, \tilde{\alpha}, \tilde{\beta}, \tilde{\gamma}) = \frac{\varepsilon - 1}{2} + \frac{\tilde{\gamma}(1 + \varepsilon)}{2\tilde{\alpha} + \tilde{\beta}};$$

$$\zeta(\varepsilon, \tilde{\alpha}, \tilde{\beta}, \tilde{\gamma}) = \frac{-4(\tilde{\alpha} - \tilde{\gamma})^2 + \tilde{\beta}(4\tilde{\alpha} + 4\tilde{\gamma} - 3\tilde{\beta}) + \varepsilon[2(\tilde{\alpha} + \tilde{\gamma}) + \tilde{\beta}]^2}{4[2(\tilde{\alpha}^2 + \tilde{\gamma}^2) + \tilde{\beta}^2]} \quad (12)$$

Substitution of equation (12) into equations (7) and (9) involves rather intricate expressions that are hardly appropriate here. The force constants can be directly evaluated making use of these algebraic expressions supplemented, for example with the relations for the local vibration intensities in the first coordination sphere $\mu_1 = P_1^2(\lambda_l)\mu_0$. Note, μ_1 is a measurable quantity.

Now we turn to the discussion of the formation of the fcc(111) (close-packed) surface in a crystal, e.g. such as Ag. In this case, the change in the force interaction between the surface atoms is negligible, and the interaction of the surface atoms with the atoms of the subsurface layer may be considered as central

$$\Phi_{ik}^{(S)}(\mathbf{r}, \mathbf{r}^{(S)} + \Delta^{(SubS)}) = \alpha_0 \frac{\Delta_i^{(SubS)} \Delta_k^{(SubS)}}{|\Delta^{(SubS)}|^2}.$$

The parameters η and ζ have the form

$$\eta(\varepsilon, \alpha_0) = \frac{4\gamma - 2\alpha + \varepsilon[2(\alpha + \gamma) + \beta]}{2(\alpha + \alpha_0 - \gamma)},$$

$$\zeta(\varepsilon, \alpha_0) = \frac{16\alpha\gamma + 4\beta(\alpha + \gamma - \beta) - 8\alpha_0^2 + \varepsilon[2(\alpha + \gamma) + \beta]^2}{2[2(\alpha - \gamma)^2 + \beta^2 + 4\alpha_0^2]} \quad (13)$$

for the displacement of the surface atom along the normal to the surface and

$$\eta(\varepsilon, \alpha_0) = \frac{2\gamma - \alpha_0 + 2\varepsilon[2(\alpha + \gamma) + \beta]}{4\alpha + 2\beta + 2\gamma + \alpha_0},$$

$$\zeta(\varepsilon, \alpha_0) = \frac{4(\alpha\beta + \alpha\gamma + \beta\gamma) - \beta^2 - 2\alpha_0^2 + \varepsilon[2(\alpha + \gamma) + \beta]^2}{2[(\alpha - \gamma)^2 + \alpha^2 + \beta^2 + \gamma^2 + \alpha_0^2]} \quad (14)$$

in the case the displacement along the surface.

Similarly, we have

$$\eta(\varepsilon, \alpha_0) = \frac{-2\alpha - \beta + 6\gamma - 4\alpha_0 + 2\varepsilon[2(\alpha + \gamma) + 4\beta]}{6\alpha + 3\beta - 2\gamma + 4\alpha_0},$$

$$\zeta(\varepsilon, \alpha_0) = \frac{4(\alpha\beta + \alpha\gamma + \beta\gamma) - 2(\alpha^2 + \beta^2 + \gamma^2 + 4\alpha_0^2) + \varepsilon[2(\alpha + \gamma) + \beta]^2}{2(\alpha - \gamma)^2 + 4\alpha^2 + 3\beta^2 + 4\gamma^2 + 8\alpha_0^2} \quad (15)$$

for the displacement of the subsurface atom along the normal to the surface and

$$\eta(\varepsilon, \alpha_0) = \frac{-2\alpha - \beta + 3\gamma - \alpha_0 + 2\varepsilon[2(\alpha + \gamma) + 4\beta]}{6\alpha + 3\beta + \gamma + \alpha_0},$$

$$\zeta(\varepsilon, \alpha_0) = \{2(3\alpha\beta + 2\alpha\gamma + 3\beta\gamma) - 2(\alpha^2 + \beta^2 + \gamma^2 + \alpha_0^2) + \varepsilon[2(\alpha + \gamma) + \beta]^2\} \{2(\alpha - \gamma)^2 + (\alpha + \gamma)^2 + 5(\alpha^2 + \gamma^2) + 3\beta^2 + 2\alpha_0^2\}^{-1} \quad (16)$$

for the displacement of the atom along the surface.

With the help of equation (8) and (13)–(16) we find the parameters α_0 and ε that specify conditions under which LVS exist. The Al impurity in Ag causes LVS in all of the cases shown in figure 2.

The local frequencies ω_l/ω_m , where according to [26] $2\pi\omega_m \approx 5.537$ THz, along with their intensities at the

impurity μ_0 and in the first coordination sphere μ_1 are displayed in figure 3 as functions of the parameter α_0 for an Al impurity in Ag. Solid lines represent the calculations using equations (7), (9), and (13)–(16). The points on the curves indicate the calculated poles of the functions $\tilde{G}_{(76)}(\lambda, \alpha_0, \varepsilon)$ and the residues at these poles. Figure 3 demonstrates the acceptable agreement between the analytical and exact numerical calculations for frequencies and intensities of LVS.

4. Conclusions

The method proposed, for constructing analytical approximations for the basic characteristics of LVS, is shown to be effective and accurate in calculations of the frequencies and intensities of LVS caused by defects, such as near-surface impurities. Analytical approximations for LVS due to impurities near the other boundaries of the sample, e.g. near surfaces with other orientations, ribs and vertices, and in the vicinity of vacancies [29] can be derived with the approach developed. These analytical approximations provide us with useful and versatile tools to deduce the parameters of the host crystal and its defect structure from frequencies and other characteristics of LVS obtained in experiments.

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