INFLUENCE OF THE FINITE DEFORMATIONS CHANGING THE SYMMETRY OF AN INITIAL LATTICE ON A GENERATION OF ATOMS DISPLACEMENTS WAVES BY NON-EQUILIBRIUM ELECTRONS

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Abstract

For the model electronic spectrum in the tight-binding approximation it is shown that the finite homogeneous deformation essentially increases the quantity of pairs of electronic states which are active in generation of atoms displacement waves. This conclusion gives additional possibilities for the explanation of features of the process of martensitic transformation.

The process of generation of atomic displacement waves is energized by stimulated emission of phonons during transitions of the non-equilibrium 3d-electrons between the inversely occupied states. The microscopic theory of generation of waves controlling the martensite crystal growth (without taking into account deformation of a lattice) is in detail stated in [1]. The interphase region is characterized by the considerable chemical-potential gradient \( \nabla \mu \). It is considered that chemical-potential gradient \( \nabla \mu \) of electrons is defining the non-equilibrium degree. For simplicity of analysis it is assumed that \( \nabla \mu \) exists in all volume. At the analysis of generation conditions such assumption is comprehensible inasmuch as the interphase region width (on the stage of growth of crystal) exceeds the lattice parameter on two or three order [1]. The initial inverse of population of pairs of electronic states \( \sigma_0 \) is proportional to \( \nabla \mu \).

The condition of generation is resulted in a reference view:

\[
\sigma_0 > \sigma_{th}, \quad \sigma_{th} = \frac{\Gamma \kappa |W|^2 R_{ef}}{\text{Ref}}.
\] (1)

In (1) \( \sigma_{th} \) - threshold value of an inverse populations difference, which is proportional to the inherent attenuation \( \Gamma \) of radiating electrons, as well as to the rate of damping \( \kappa \) of generation phonons and inversely proportional to the square of the matrix-element \( W \) of electron-phonon interaction, as well as to the number of pairs of equidistant electronic states \( R_{ef} \).

The calculation of \( R_{ef} \) has an important significance as the execution (1) is possible only for the large values of \( R_{ef} \). In the quasi-momentum space \( s \)-surfaces separate pairs of inversely populated electronic states, on which convert in a zero projections of group speed of electrons with quasi-momentum \( k \) on a direction of spatial heterogeneity [2]. The equation for the \( s \) - surfaces is specified by the
condition of conversion in zero of the scalar product of velocity and chemical-potential gradient vectors

\[ (\mathbf{v}, \nabla \mu) = 0. \]  

(2)

It is interesting to calculate the \( R_{ef} \) in an actual region of energies \( \Delta \) of the order 0.1 eV in a vicinity of Fermi-level \( \mu \). Hence it is necessary to find the area \( \Delta S \) of s-surface portions located between the isoenergetic surfaces \( \varepsilon = \mu \pm \Delta \) and to take into account that \( R_{ef} \sim \Delta S \). An important stage that provides qualitative consideration and required estimation is the case of an electron energy spectrum in the tight-binding approximation for BCC and FCC lattices [3]. The point is that an analytical form of a spectrum allows to immediately establish an analytical form for an electron velocity field. Knowing the field one can find the s-surfaces.

It is clear, that usage of electronic spectrum of a non-deformed (ideal) lattice is possible for small deformations and, basically, such usage is excused at the description of threshold deformation \( \leq 10^{-3} \) (about an elastic limit). However the question about an evolution of \( R_{ef} \) during transformation is open. Let’s notice, that the large values of \( R_{ef} \) are connected to electronic states having the energies \( \varepsilon \approx \varepsilon_p \) where \( \varepsilon_p \) is a peak of the density of states (DOS). The deformation should lead to displacement of a position \( \varepsilon_p \) relatively of the Fermi-level \( \mu \). For the symmetric peak of DOS not changing the form during deformation it would be possible to expect that the value \( R_{ef} \) will increase at the decreasing of \( |\varepsilon_p - \mu| \), whereas the value \( R_{ef} \) will decrease at the increasing of \( |\varepsilon_p - \mu| \). It is easy to present a non-monotonic behavior of \( R_{ef} \), when during deformation the peak of DOS is displaced from a position above (below) the Fermi-level in a position below (above) the Fermi-level. Then \( R_{ef} \) achieves a maximum at \( \varepsilon_p \approx \mu \). Let’s remind that \( \gamma - \alpha \) (fcc - bcc) martensitic transformation is a classical example of reconstructive transformation. This transformation is characterized by finite deformation (Bein’s deformation [4]) which onto two order exceeds the threshold deformation. Therefore it is interesting to consider the influence of deformation \( \varepsilon \sim 0,1 \).

The threshold deformation at \( \gamma - \alpha \) martensitic transformation as the basic components contains deformation of a stretching along an axis of symmetry of the fourth order initial fcc lattice. Therefore it is expedient to consider influence on \( R_{ef} \) of the one-axis deformations of a stretching. Let’s designate deformation value \( \varepsilon_1 \), then we can write the elementary modified electron energy spectrum in the tight-binding approximation:

\[
E(k) = E_0 - 4E_1 \left( \cos \eta_1 \cos \eta_2 + \frac{2}{1 + (1 + \varepsilon_1)^2} \cos \eta_3 (1 + \varepsilon_1) [\cos \eta_1 + \cos \eta_2] \right), \tag{3}
\]
where $E_0$ is the atomic energy level; $E_1$ is the parameter characterizing interaction with the first neighbors without strain; $\eta_i = a k_i/2$; $a$ is the lattice parameter; and $i = 1, 2, 3$. It is considered also, that, according to [5], $E_1$ is inversely proportional to a square of distance between the nearest neighbors. In [3] a change of these distances at deformation is taken into account. The direction $\mathbf{e}$ is collinear to axis of a stretching. The given case is the most simple for an interpretation of dependence $R_{ef}$ on deformation. Really, in the density of states corresponding to a spectrum, there is a unique peak. Displacement and change of the form of this peak during deformation are automatically calculated. Also all sheets of $s$-surfaces at the specified direction $\mathbf{e}$ are flat and their contribution in $\Delta S$ can be calculated in an actual region of energy.

Figure 1 demonstrates the change of peak of DOS during deformation.

![Figure 1](image-url)

**Figure 1.** Evolution of peak of DOS during deformation for a spectrum at $E_0 = 0$ and $E_1 = 0$, 3125 eV: a) $\varepsilon_1 = 0$; b) $\varepsilon_1 = 0$, 1; c) $\varepsilon_1 = 0$, 12; d) $\varepsilon_1 = 0$, 2.

From fig[1] it is visible, that: the peak of DOS is asymmetrical; the peak height decreases at the growth of $\varepsilon_1$; the peak of DOS localized near the zone top is displaced in a direction to the center of the zone and is broadened. Let’s note, that during deformation Fermi-level $\mu$ also experiences the displacement to centre of a zone, however the rate of change of $\mu$ is noticeably lower, than the rate of change of $\varepsilon_p$. On fig[2] the dependence on deformation of dimensionless area $\Delta S(\varepsilon_1)/\Delta S(0)$ of a $s$-surface portion is demonstrated for an energy interval $(0, 6 \div 1, 0)$ eV, i.e.
The analysis shows that the essential increment of area $\Delta S(\varepsilon_1)/\Delta S(0)$ in the strain interval $0.06 \div 0.4$ (the greatest growth of rate of $\Delta S(\varepsilon_1)/\Delta S(0)$ is achieved in narrow region $0.103 < \varepsilon_1 < 0.116$) is caused by the states located on square planes of Brillouin zone (orthogonal to $\mathbf{e}$). The area of this square planes increases during deformation. At $\varepsilon_1 < 0.06$ the states on these planes have a weak dispersion and lay above an interval $(\mu - \Delta, \mu + \Delta)$. For $\varepsilon_1 > 0.06$ a part of states starts to get into an energy interval $(\mu - \Delta, \mu + \Delta)$. Their quantity achieves of a maximum at $\varepsilon_1 \approx 0.3$. Let’s notices that the peak lays above the Fermi-level at $\varepsilon_1 < 0.26$ ($\varepsilon_p - \mu > 0$) and at $\varepsilon_1 > 0.26$ lays under the Fermi-level ($\varepsilon_p - \mu < 0$). The non-monotone behavior of $\Delta S(\varepsilon_1)/\Delta S(0)$ as a whole is compounded with
expected behavior. Really without taking into account of dependence of \( \mu \) on \( \varepsilon_1 \) the condition \( \varepsilon_p \approx \mu \) is realized at \( \varepsilon_1 \approx 0, 25 \) and \( \varepsilon_1 \approx 0, 3 \) corresponds to a maximum of \( \Delta S(\varepsilon_1)/\Delta S(0) \). Taking into account the lowering of \( \mu \) during deformation the condition \( \varepsilon_p \approx \mu \) can be executed for \( \varepsilon_1 > 0, 44 \). The maximum \( \Delta S(\varepsilon_1)/\Delta S(0) \) corresponds to value \( \varepsilon_1 \approx 0, 46 \). Thus, taking into account of dependence of \( \mu \) on \( \varepsilon_1 \) we obtain that the difference of values of \( \varepsilon_1 \) corresponding to condition \( \varepsilon_p \approx \mu \) and the requirement \( \Delta S(\varepsilon_1)/\Delta S(0) = (\Delta S(\varepsilon_1)/\Delta S(0))_{max} \) decreases (this difference does not access in a zero, as the peak of DOS is not symmetric).

**Final remarks**

1. As it was discussed in [1], the interphase region width has value that is approximately equal \( \lambda/2 \), where \( \lambda \) is the wave length corresponding to a characteristic interval \((0, 1 \div 1) \mu m\) in a hypersound range. It is clear, that electronic states being active in wave generation should have a weak dispersion. It is possible to consider [3] that velocity \( v_k \) of such electrons is close to their velocity of drift \( v_d \) and approximately is equal to \( 10^4 \) km/s. Then the possible contribution to attenuation \( \Gamma \) in (11) caused by occurrence of additional heterogeneity scale of, does not exceed (in units of frequency) \( \sim 10^{12} \) s\(^{-1}\). Inasmuch as such \( \Gamma \) is being in the consent with the experimental data for samples in absence of the deformation [1] it is natural to expect that deformations is influenced, mainly, on \( R_{ef} \). It is clear that in this case a dependence \( R_{ef}(\varepsilon_1) \) gives dependence \( \sigma_{th}(\varepsilon_1) \).

2. The considered example testifies about an opportunity of essential decrease of threshold value \( \sigma_{th} \) during deformation. This conclusion is important for the description of a stage of growth of the crystal of martensite (when the lattice experiences the significant deformation after loss of stability) as well as for the description of the nucleation stage of martensitic crystals. It is gives additional arguments in favor of the mechanism of rigid excitation of initial fluctuations at reconstructive martensitic transformations (\( \sigma_{th} \) is decreasing when the amplitudes of fluctuations are increasing).

3. It is possible to assume, that most intensive martensitic transformations take place in alloys of such composition for which the decreasing of \( \sigma_{th} \) is typical during increasing deformation.

**References**

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