# Mechanism of martensitic transformation due to the disequilibrium of the electron-phonon system

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It is proposed to regard martensitic transformations that proceed at finite temperature-variation rates as the consequence of stimulated emission of acoustic phonons by electrons. The conditions for phonon generation in transitions of the electrons between states with maximum inverted population are analyzed.

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The martensitic transformation (MT), which is a diffusionless process of lattice restructuring, is realized in steels and in many transition metals and their alloys. In a typical situation, the cooling of the sample surface (quenching) in the direct MT or the heating in the inverse MT are carried out at finite rates.

A metal (assumed for simplicity to be paramagnetic) is a non-equilibrium system of interacting electrons and phonons. The degree of disequilibrium is determined by the local temperature gradient $\nabla T(\mathbf{r},t)$, which depends in general both on the radius vector $\mathbf{r}$ and on the time $t$. Assuming the band description to be valid, we denote by $f_{j\mathbf{p}}$ the non-equilibrium distribution function of the electrons in the state $(j\mathbf{p})$, where $j$ is the number of the band and $\mathbf{p}$ is the quasimomentum of an electron with $\epsilon_{j\mathbf{p}}$. At $\nabla T \neq 0$ there exist electronic states with inverted populations, the maximum population inversion being realized between states of electrons with antiparallel momenta $p'\uparrow\downarrow p$ directed along and against $\nabla T$. This is illustrated in Fig. 1, which shows the equilibrium ($f^0_{\mathbf{p}}$) and non-equilibrium ($f_{\mathbf{p}}$) functions (see § 3.1 in[1]):

$$f^{\circ}_{\mathbf{p}} = \left\{ \exp\left[\frac{\epsilon_p - \mu}{kT}\right] + 1 \right\}^{-1}, \qquad f_{\mathbf{p}} - f^{\circ}_{\mathbf{p}} \approx \frac{\partial f^{\circ}_{\mathbf{p}}}{\partial \epsilon_{\mathbf{p}}} \frac{(\epsilon_{\mathbf{p}} - \mu)}{T} \vec{\Lambda}_{\mathbf{p}} \vec{\nabla} T, \tag{1}$$

where $\mu$ is the Fermi level and $\vec{\Lambda}_p$ is the vector mean free path of the electron with quasimomentum $\mathbf{p}$. From the standard kinetic equation for the phonon distribution function (see § 1.1 and § 1.14 in[1]) it follows that the transitions of electrons between states $(i\mathbf{p}')$ and $(j\mathbf{p})$ with inverted populations lead to generation of longitudinal acoustical phonons with $h\nu_q$ if

$$f_{i\mathbf{p}'} - f_{j\mathbf{p}} > 0 \tag{2}$$

and the following conversion laws are satisfied

$$\epsilon_{i\mathbf{p}'} - \epsilon_{j\mathbf{p}} - h\nu_{\mathbf{q}} = 0, \qquad \mathbf{p}' - \mathbf{p} - \mathbf{q} = 0, \mathbf{Q}, \tag{3}$$

where equality to zero or to the reciprocal-lattice vector $\mathbf{Q}$ corresponds to the normal scattering process $N$ or to the umklapp process $V$.

It is seen from Fig. 1 that the transitions of electrons above and below the Fermi level ($\epsilon_{\mathbf{p}'}\epsilon_{\mathbf{p}} > \mu$ and $\epsilon_{\mathbf{p}'},\epsilon_{\mathbf{p}} < \mu$) can lead to generation of phonons with quasimomenta $\mathbf{q}$ parallel and

  

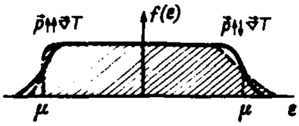

FIG. 1. Electron distribution functions $f_p^0$ at $\nabla T = 0$ (solid line) and $f_p$ at $\nabla T \neq 0$ (dashed line).

antiparallel to $\vec{\nabla} T$, respectively. However, realization of the generation, which calls for compatibility of conditions (2) and (3), at real values of $\nabla T$ is possible not at arbitrary positions of the Fermi level. Assuming $h\nu_q (kT)^{-1} \ll 1$, which holds for frequencies $\nu_q \lesssim 10^{10}$ Hz all the way to $T = 5°$, we represent the generation condition (2), with (1) and (3) taken into account, in the form

$$2|\vec{\Lambda}\vec{\nabla} T| T^{-1} - \tau_{tr} > 0, \qquad \tau_{tr} = h\nu_q (|\epsilon_{p'} - \mu|)^{-1}(1 + |\vec{\Lambda}\vec{\nabla} T| T^{-1}), \tag{4}$$

where $\vec{\Lambda} = \vec{\Lambda}_p \approx -\vec{\Lambda}_{p'}$. Let us estimate the range of generated frequencies. Assuming $|\epsilon_{p'} - \mu| \approx kT, T = 300°$, $\Lambda = 10^6$ deg/cm (large temperature-variation rates), we get from (4) $0 < \nu_q < 10^{10}$ Hz. This means that even at large $T$ the largest of the frequencies $\nu_q$ corresponds to a wave number $q$ which is smaller by two or three orders of magnitude than $q_{max}$ on boundary 1 of the Brillouin zone ($\nu_{q_{max}} \approx 10^{12}$–$10^{13}$ Hz). It follows then from the momentum conservation law that phonon generation in transitions of electrons between the states $\mathbf{p}' \uparrow\downarrow \vec{\nabla} T$ and $\mathbf{p} \uparrow\uparrow \vec{\nabla} T$ is possible both via $N$ and $V$ processes, if the Fermi level lies near the bottom or near the top of the electron band. Both possibilities can be easily realized in transition metals and their alloys (this explains why MT are typical in them) at $d \to d$ (or $f \to f$ for rare earths) transitions of the electrons, since the $d$ (or $f$) bands are narrow and intersect with the Fermi level. The participation of $s \to s$ and $d \to s$ ($f \to s$) transitions in the generation of phonons is less typical and is most probable for those reciprocal-space directions in which the $s$ band is narrow. These transitions can be only of type $V$ (the bottom of the $s$ band is always substantially lower than $\mu$) and are due to the anisotropy of the energy spectrum of the $s$ electron.

Thus, MT can be regarded as the consequence of phonon generation in the course of a non-equilibrium variation of the temperature of the initial phase. The transition to the generation regime, in analogy with laser emission, is interpreted according to Haken (see the Appendix of[2]) as a second-order phase transition for the radiation field, and is due to the appearance of nonzero displacement-wave amplitudes. A martensitic transformation that proceeds as a rule with clearly pronounced attributes of a first-order transition is realized when these amplitudes reach threshold values after a certain threshold time following the start of cooling or heating (the condition of thermodynamic instability of the phase that undergoes the MT is asssumed satisfied[3].)

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[1]B.M. Mogilevskiĭ and A.F. Chudnovskiĭ, Teploprovodnost' poluprovodnikov (Thermal Conductivity of Semiconductors), Nauka, 1972, §1.1, §1.14, §3.1.
[2]M. Lax, transl. in: Fluktuatsii i kogerentnye yavleniya (Fluctuations and Coherent Phenomena), Mir, 1974, p. 277.
[3]M.P. Kashchenko and R.I. Mints, Fiz. Tverd. Tela **19**, 329 (1977) [Sov. Phys. Solid State **19**, 189 (1977)].