Possible mechanism for laser annealing

I. M. Suslov
P. N. Lebedev Physics Institute, Academy of Sciences of the USSR, Moscow

(Submitted 14 February 1984; resubmitted 7 May 1984)
Pis'ma Zh. Eksp. Teor. Fiz. **39**, No. 12, 547–550 (25 June 1984)

Laser bombardment of the surface of a semiconductor excites relative oscillations of two sublattices of the crystal with an amplitude on the order of the interatomic distance. These oscillations may be the reason for laser annealing.

The laser bombardment of the surface of a semiconductor eliminates the defective layer from the surface and produces a perfect crystalline structure: a "laser annealing" occurs. Nonthermal models of the laser annealing have recently been discussed widely.[1,2] The most important is the model recently proposed by Kapaev *et al.*,[3] according to which the laser annealing results from a Peierls transition from an insulator to a metal and back. In the present letter we show that a curious effect would occur according to this model, and this effect may play a governing role in laser annealing.

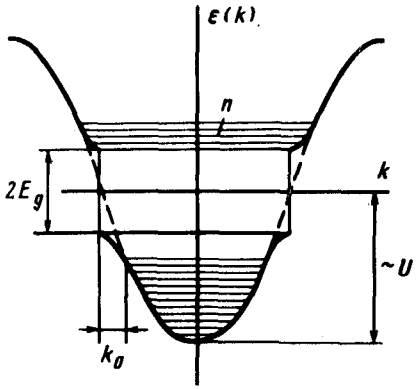

FIG. 1.

We consider a *bcc* metal, which we describe in the strong-binding approximation, taking nearest neighbors into account (the band width is $\sim U$). With a half-filled band the Fermi surface is an exact cube, and the system is unstable with respect to a relative displacement of two cubic sublattices along a main diagonal. A gap of width $2E_g^0$ opens up at the Fermi level, and the system becomes an insulator.[4] To analyze the laser annealing of such an insulator, we assume (ω_D is the Debye frequency)

$$\hbar\omega_D \ll E_g^0 \ll U. \tag{1}$$

During the laser pumping some of the electrons are scattered across the gap; an electron gas of density n forms above the gap, and we assume that it is degenerate (Fig. 1). The potential energy of the system is the sum of the energy of the electron gas, V_e, and the elastic energy (V_{el}) due to the covalent binding:

$$V = V_e + V_{\text{el}}, \quad V_{\text{el}} = \frac{1}{2}kx^2$$

$$V_e(E_g) = V_e(0) + 2N(\epsilon_F)\left\{\int_0^U d\epsilon\,(\epsilon - \sqrt{\epsilon^2 + E_g^2}) + 2\int_0^\Delta d\epsilon\sqrt{\epsilon^2 + E_g^2}\right\}, \tag{2}$$

where x is the relative displacement of the sublattices, U is a cutoff parameter (on the order of the band width), $\Delta = v_F k_0 \sim U^n/n_0$, k_0 is defined in Fig. 1, n_0 is the total electron density, $N(\epsilon_F)$ and v_F are the state density and Fermi velocity in the metallic phase (with $E_g = 0$), and the spectrum $\epsilon(\mathbf{k})$ near the gap is chosen in the weak-binding approximation. Since $E_g \sim |x|$, the curves of $V(x)$ for various values of n have the form shown in Fig. 2.

At $n = 0$ (curve 1), the insulating state is stable ($x = x_0$, point A), while the metallic state ($x = 0$, point A') is absolutely unstable. At nonzero values of n (curve 2) the metallic state becomes metastable; finally, at $n > n_c$ (curve 3), where

$$n_c = \frac{3}{3\sqrt{3}}N(\epsilon_F)E_g^0 \sim n_0 E_g^0/U, \tag{3}$$

the insulating state becomes absolutely unstable.[3]

Let us examine the dynamics of the system after illumination by an intense laser pulse of very short duration (shorter than ω_D^{-1}). By the end of the laser pulse the

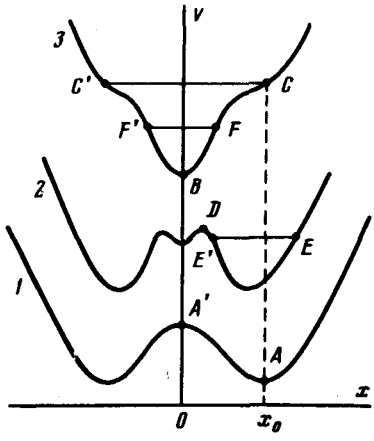

FIG. 2.

system has gone from the original state A to state C, and the system has begun to move freely. Inertia keeps the system from sliding immediately into state B, and it begins to oscillate between C and C'. Since these oscillations correspond to a relative motion of the two sublattices, their frequency is $\sim\omega_D$, and the damping is determined by the expressions for the absorption coefficient for short-wavelength sound:

$$\gamma \sim \omega_D T/U_b \ll \omega_D \qquad (T \gtrsim \hbar\omega_D).$$

This damping is slight, on the order of the parameter T/U_b, where U_b is the binding energy of the lattice. Recombination of the carriers causes the parameters of the oscillatory system to change: The system goes from curve 3 to curve 2 and then to curve 1. This change is slow, however, since the times τ_{rec} for many-phonon and Auger recombination are large in comparison with ω_D^{-1}. Near the point $x = 0$ the gap width E_g is small, and recombination can result from single-phonon processes. The rate of this recombination is determined by the energy relaxation time

$$\tau_E \sim \omega_D^{-1} E_g^0/\hbar\omega_D \gg \omega_D^{-1} \tag{4}$$

(during the emission of a phonon ω_D^{-1}, the electron energy changes by $\hbar\omega_D$, while its average value is $\sim E_g^0$ at $n \sim n_c$) and is also small. Furthermore, states with a small gap ($E_g \lesssim \hbar\omega_D$) are traversed in a small fraction of a period.

We thus have an oscillatory system with a large Q. We will show that in the case of long laser pulses there can be a parametric pumping, and the system can operate as an oscillator. We assume the following conditions:

$$(J\alpha/\hbar\omega_0)\tau_{\text{rec}} \gtrsim n_c, \tag{5}$$

$$(J\alpha/\hbar\omega_0)\tau_E \ll n_c, \tag{6}$$

$$U_b \gg T \gtrsim T_0, \quad T_0 \sim E_g^0(E_g^0/U)(J\alpha\tau_E/\hbar\omega_0 n_c)^4, \tag{7}$$

where J is the energy flux density of the light, $\hbar\omega_0$ is the photon energy, α^{-1} is the

damping length, and $J\alpha/\hbar\omega_0$ is the density of electrons which are scattered across the gap per unit time. The length of the pulse is irrelevant if the sample is not overheated.

Conditions (5)–(7) are the conditions for self-excitation of the system. The insulating state (the point A) is unstable, since the carrier density n increases above the critical point according to (5). The metallic state (the point B) is unstable, since at $E_g = 0$ the recombination is determined by the time τ_E, and the carrier density n drops nearly to zero by virtue of (6). The system is not retained in the shallow minimum at $x = 0$ at small values of n because of the inequality at the right in (7). The inequality at the left in (7) is the condition for a high Q.

A periodic motion is also possible over a broad range of the density n. At small values of n this periodic motion occurs in the upper part of the insulator well (trajectory EE'), while at large values of n it occurs near the metallic state (FF'). Trajectory EE' is chosen from the condition that the number of carriers which have recombined near the point E' (at E' the condition $E_g \lesssim \hbar\omega_D$ holds) is replenished by the laser pumping during the period of the motion. This choice is always possible, since the time taken to pass through the neighborhood of the point E' depends strongly on the position of the trajectory: This time becomes infinite as E' approaches D. It is easy to see that there exists a strong feedback; for example, when trajectory EE' in Fig. 2 is deflected downward there is a sharp decrease in the time taken to cross the region of rapid recombination near E', and the number of carriers increases on the average over a period. As a result, the maximum of the potential energy at D decreases, and there is an increase in the time taken to traverse the vicinity of the point E'.

For the trajectory of FF' a downward deflection in Fig. 2 leads to a relative increase in the time taken to cross the region $x \approx 0$ (in comparison with the period of the motion), and there is a decrease in n. Since the potential energy in this region is of the form

$$V(x) \sim x^2 \ln |x_1/x|, \quad x \ll x_1, \quad x_1 \sim n^2,$$

a decrease in n leads to an increase in the width of the potential well and to a decrease in the relative time taken to cross the region $x \simeq 0$.

In summary, undamped oscillations of two sublattices with respect to each other, with an amplitude on the order of the interatomic distance, are excited during laser bombardment. Such a severe "shaking" can "heal" defects and cause a macroscopic redistribution of impurities. Because of the coherent nature of this shaking, the interstitial atoms move in a periodic field (periodic over time and space) and can have a range considerably greater than the lattice constant. Accordingly, the diffusion coefficients are greater than in a liquid phase (the acceleration of diffusion as a result of a "radiative shaking" of a different origin was discussed by Indenbom[5] and has been confirmed experimentally).[6] In certain cases, an annealing may not occur, and the crystal may instead be rendered amorphous.

The effect predicted here may be observed in semiconductors with small values of E_g^0 near the Peierls structural transition if there is good heat removal (e.g., in superfluid helium) and at an optimum choice of light frequency. This effect might be exploited to develop an "acoustic laser."

I wish to thank A. F. Andreev, Yu. V. Kopaev, and V. B. Stopachinskiĭ for discussions.

[1]J. A. Van Vechten *et al.*, Phys. Lett. **A74**, 417, 422 (1979).
[2]J. A. Van Vechten, Solid State Commun. **39**, 1285 (1981).
[3]V. V. Kapaev, Yu. V. Kopaev, and S. N. Molotkov, Mikroélektronika **12**, 499 (1983).
[4]R. Peierls, Quantum Theory of Solids, Oxford Univ. Press, London, 1955 (Russ. transl., Mir, Moscow, 1956).
[5]V. L. Indenbom, Pis'ma Zh. Tekh. Fiz. **5**, 489 (1979) [Sov. Tech. Phys. Lett. **5**, 200 (1979)].
[6]É. D. Aluker, V. V. Gavrilov, S. A. Chernov, and S. S. Étsin, Fiz. Tverd. Tela (Leningrad) **26**, 321 (1984) [Sov. Phys. Solid State (to be published)].

Translated by Dave Parsons
Edited by S. J. Amoretty