Local phonon vibrations

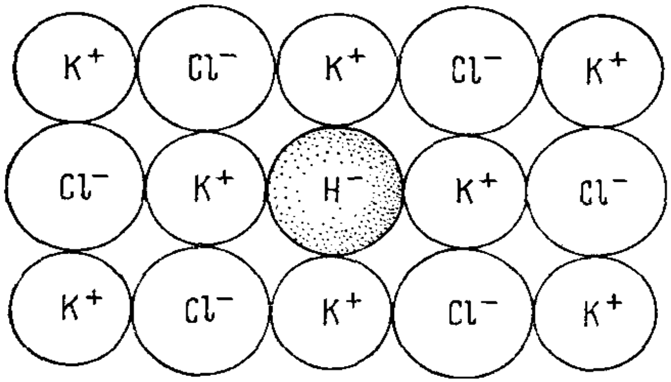
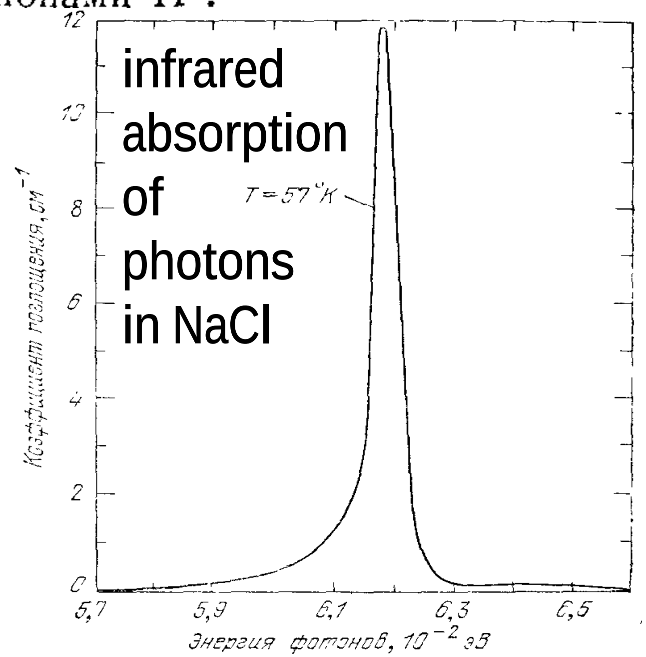


Рис. 5.26. Ион H^-, заместивший ион Cl^- в кристалле KCl; такой примесный центр называется U-центром. Высокочастотные локальные фононные колебания обусловлены ионами H^-.

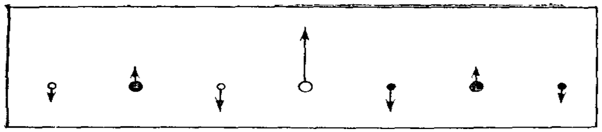


The simplest problem in which a local phonon is considered is a linear chain of atoms, in which all atoms except one have mass M, and one atom has mass M' < M. Let us show that one of the normal vibrations of the lattice is localized in the region of a light atom and the corresponding frequency is greater than ω_{max} of the undisturbed (unperturbed) lattice. We take into account the interaction of only the nearest neighbors and assume that this interaction is the same for both atoms M' and M, and for atoms M and M. Let's place the light atom at the origin, s=0. The equations of motion for the lattice have the form

$$M' \frac{d^2 u_0}{dt^2} = C\,(u_1 + u_{-1} - 2u_0),$$

$$M \frac{d^2 u_1}{dt^2} = C\,(u_2 + u_0 - 2u_1), \quad \text{и т. д.}$$

Local phonon vibrations (2)



The equations of motion for a 1D lattice are:

$$M' \frac{d^2 u_0}{dt^2} = C(u_1 + u_{-1} - 2u_0), \quad (1)$$

$$M \frac{d^2 u_1}{dt^2} = C(u_2 + u_0 - 2u_1), \text{ и т. д.} \quad (2)$$

We are looking for a solution in the form of an exponentially decaying (as we move away from s = 0) function, which in the limit M'--> M approaches the form of a normal oscillation of the maximum frequency for an unbroken lattice:

$$u_s = u_0 (-1)^s e^{-i\omega t} e^{-|s|\alpha}$$

Substituting this solution to Eq. (2) we obtain $\omega^2 = (C/M)(2 + e^{-\alpha} + e^{\alpha})$,

while its substitution to Eq. (1) gives $\omega^2 = (C/M')(2 + 2e^{-\alpha})$.

These equations are compatible if $e^{\alpha} = (2M - M')/M'$, ⇒

the frequency of local phonon mode $\omega^2 = \omega_{max}^2 \frac{M^2}{2MM' - M'^2}$

If M'<< M, $\omega^2 = \omega_{max}^2 (M/2M')$

The solution at the boundary of Brillouin zone for an unperturbed lattice has the form

$$u_s = u(0) \cos s\pi\, e^{-i\omega t} = u(0)(-1)^s e^{-i\omega t}$$ **где** $\omega_{max} = (4C/M)^{1/2}$