Thermal excitation of trapped electron

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Observing, in this report, that the quantitative insufficiency of Maxwell-tail model[1] of TSEE (thermally stimulated exoelectron emission), which has hitherto been scarcely investigated, has its source in the method itself of dealing with an elementary problem of thermal excitations of trapped electrons, we wish to point out some problems in there.

The characteristic features of TSEE for alkalihalide irradiated with ionizing radiation are;

(i) The trap depth for thermal excitation is considerably deep compared with that of semiconductors in which thermal excitations of trapped electrons is usually observed at R. T.[2]

(ii) The effective temperature of exoelectrons measured from their kinetic energies is about one figure higher than the temperature of thermal equilibrium in crystals.[3]

Previous investigations of TSEE were phenomenological, and there were only qualitative explanations also for the above two features.

We here will not take up Case (ii) in detail decause the apparent accelerating process just stated is experienced by electrons elevated to conduction band by thermal stimulation and then migrated to the surface, which may be regarded as second stage for the mechanism of TSEE.

There has been suggested two possibilities resulting for this apparent accelerating process.

One is the negative electron affinity observed in the case of LiF[4] and the other is the conductionband's bending at the surface[5] of the crystal due to the lattice relaxation, some defects, adsorption and any other reasons.

We shall therefore consider Case (i).

Irradiated alkalihalide shows characteristic glowpeaks of TSEE and their traps

are regarded as differing in kind, location and manner of stimulation, in particular the "F" glowpeak is considered to be due to F center[6]. We therefore consider the F glowpeak here.

In case of well-investigated F glowpeak of TSEE for LiF, the trap depth is 1.42eV[2], the peak temperature is 580K[6] with its thermal energy of 48 meV, and the optical absorption energy of the F center is 3.1 eV. These data suggest for the mechanism producing the F glowpeak that trapped electrons at F centers in bulk pass through the thermal potential barrier, which is considerably lower than the optical potential barrier for stimulation, and then through an apparent accelerating process at the surface to be excited into the vacum level.

The Case (i) induces an important question why the trapped electron can pass through such a high barrier by only thermal stimulation.

So far, concerning thermal stimulation of trapped electrons resulting for TSEE, its rate process has been considered to be explained qualitatively by Maxwell-tail model which states that the conduction electron having energy as high as electron affinity is emitted by thermal stimulation with assuming quasi-thermal equilibrium.

However, this model can not explain the experimental values, though it gives an expression for exoelectron emission.

We shall therefore return to an elementary problem of NRT (non-radiative transition) of trapped electrons in insulator to reexamine the underlying quantum-theoretical treatment.

The thermal excitation of the trapped electron in insulator has been investigated as the problem of NRT[7,8].

We shall consider whether the theory suggested by Toyozawa[7] is applicable or not for the deeply trapped electron.

The assumptions underlying in the paper are the following:

(i) The lattice vibration is hermonic while the normal coordinate is of the perfect crystal, which supposes that only LO mode interacts with the excess electron in insulator through Fröhlich Hamiltonian without considering the localization of F electron.

(ii) The electron-phonon interaction is described by linear approximation with respect to the normal coordinate of the lattice vibration.

(iii) "Non-adiabatic term "(*ie.* the deviation from adiabatic approximation in electron-phonon system) is regarded as perturbation.

Under these assumption he has shown the following expression for NRT pro-

bability of the trapped electron;

$P=(2\pi)^{7/2}\hbar^{-3}\gamma^{-1/2}S^*S\ (\beta\varepsilon_0)^{-1/2}\exp(-\beta\varepsilon^*)$,

where γ is the interaction strength between the electron and phonon, S*S is NRT probability, ε_0 is thermal excitation energy, ε^* is the thermal activation energy.

This reult indicates that multiphonon of $n\approx\varepsilon_0/\hbar\omega$ is absorbed simultaneously.

Also HUANG has obtained the similar conclusion[3], applying for F absorption band of KBr and has obtained the result that 22.4 phonons are absorbed simulateneously.

Extending this result to the F glowpeak of TSEE in the case of LiF, it becomes that 17 phonons are absorbed at once.

When "non-adiabatic term" is small, from perturbation theory the thermal excitation probability per unit time can be obtained by using the phonon density matrix at thermal equilibrium.

In this case, however, the theory is applicable to only phenomena in which two or three phonons are concerned.

It therfore is rather natural to regard the theory as inapplicable for thermal stimulation of deeply trapped electrons ,*e. g.* resulting for TSEE.

More exactly, when the deviation from adiabatic approximation is so large that the electronic transition is caused by the thermal stimulation through the strong electron-phonon interaction, it might be possible that the effective temperature of the partial electron-phonon system surrounding the trapped electron differs from equilibrium temperature of the crystal.

Generally speaking, the heating process, which yield the thermal internal force and is not described by using hamiltonian, should be discussed as the problem of the transportation.

In such a case, the effective temperature of the phonon field will be described by the time-dependent function and the energy of the electron in the system will be obtained by the path integral method using a trial function containing time -dependent term.

There will appear the non-epuilibrium statistical operator in place of the density matrix mentioned above.

In fact it is recognized that there exists a formal correspondence between the non-equilibribrium statistical operator and the variational principle.[9]

We leave a detail discussion and calculation about this non-equilibrium resolution for another opportunity.

Reference

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