depend on the distortion of the lattice in the vicinity of the exciton (providing a sort of central-cell correction) that arises from the interaction of the carriers with their polarization. One therefore expects that the splitting will be larger in ionic crystals that have a strong polaron interaction than in covalent semiconductors, where the electron-phonon interaction is provided by means of the deformation potential.

Indeed, while the stress-induced splitting of the different exciton peaks is the same in Si,[1] it is different in the peaks assigned to the valley-orbit-split exciton in AgBr.[2]

In conclusion, it is pointed out that although there is no valley-orbit splitting of related indirect exciton states in the absence of the electron-phonon interaction,[3] the neglect of the latter is not, in principle, justified in the description of the creation of excitons by means of indirect optical transitions.

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Thermoelectric Power of Cu_3Au as a Function of Short-Range Order*

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A theoretical study of the diffusion thermoelectric power of Cu_3Au as a function of order above the critical temperature is made. This work is based on, and completes, our investigation on the residual resistivity of Cu-Au alloys above the critical temperature.

The diffusion thermoelectric power Q_D has been a subject of both experimental and theoretical investigation for a long time. Nevertheless, there has been practically no theoretical work done towards the study of the order dependence of Q_D of alloys. In this paper, we propose a pseudopotential theory of Q_D of binary alloys as a function of short-range order (SRO) and apply our formulation to Cu_3Au for which the reliable SRO parameters are available.[1]

Consider a disordered binary alloy with a total of N atoms of which N_A and N_B are of types A and B, respectively. Assume that these atoms are placed on a rigid Bravais lattice consisting of N sites. Further, postulate that the (pseudo)potential of the system can be written as a sum of the screened ionic pseudopotentials of types A and B, i.e.,

$$W(\vec{r}) = \sum_i \partial_i^A w_A(\vec{r} - \vec{r}_i) + \sum_i \partial_i^B w_B(\vec{r} - \vec{r}_i) , \qquad (1)$$

where the occupation operators[2] ∂_i^λ are defined as follows:

$\partial_i^\lambda = 1$ if the ith lattice site is occupied by an atom of type λ

$= 0$ otherwise

and ω_λ is the screened ionic pseudopotential of type λ.

For such a system, we have in a previous paper[3] been able to express the resistivity as a function of SRO as follows:

$$\rho(E) = \frac{3\pi m \Omega_0}{8\hbar e^2 E} \int_0^2 \left| \frac{q}{K} \langle \vec{k}+\vec{q} | w_A - w_B | \vec{k} \rangle \right|^2 \times m_A m_B \frac{q}{K} \sum_i \alpha_i C_i j(n_i q) d\left(\frac{q}{K}\right) , \qquad (2)$$

where Ω_0 is the atomic volume per ion, $m_\lambda = N_\lambda/N$, and E is the energy of an electron in the plane-wave state $|K\rangle$. The integrand appearing in Eq. (2) consists of two factors: the "atomic part," which is proportional to the square of the difference of the form factors of A and B atoms, i.e., $|\langle \vec{k}+\vec{q}|w_A|\vec{k}\rangle - \langle \vec{k}+\vec{q}|w_B|\vec{k}\rangle|^2$, and the "structural part," which is a function of short-range order parameters α_i, the coordination number of the ith shell c_i, and the vectors n_i locating the atoms in the ith shell.

The diffusion thermoelectric power in units of $\pi^2 k_B^2 \tau / 3eE$ can be written as[4]

$$Q_D = -E_F \left(\frac{\partial \ln \rho(E)}{\partial E} \right)_{E = E_F} . \qquad (3)$$

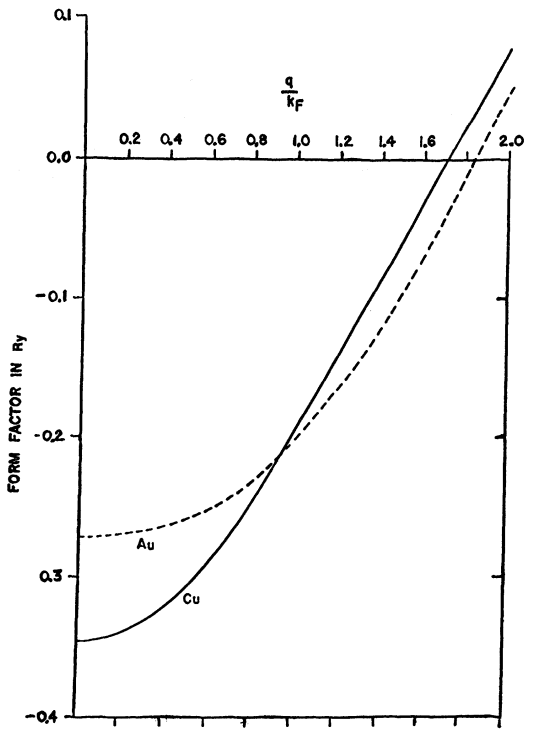

FIG. 1. Form factors of Cu and Au calculated by Animalu as a function of q/k_F based on the method of Heine, Abarenkov, and Animalu.

Substituting (2) into (3), we are led to the following result:

$$Q_D = 3 - \frac{2S(2k_F)\,|U(2k_F)|^2}{\langle SU^2\rangle} \ , \tag{4}$$

where

$$S(2k_F) = m_A m_B \sum_i \alpha_i C_i j_0(n_i\, 2k_F) \ , \tag{5}$$

$$U(2k_F) = \langle k_F + 2k_F |\, w_A - w_B \,|\, k_F \rangle \ , \tag{6}$$

and

$$\langle SU^2\rangle = \tfrac{1}{4} m_A m_B \int_0^2 \left| \frac{q}{k_F} \langle \vec{k}+\vec{q} |\, w_A - w_B \,| \vec{k}\rangle \right|^2 \times \frac{q}{k_F} \sum_i \alpha_i C_i j_0(n_i q)\, d\left(\frac{q}{k_F}\right) \ . \tag{7}$$

It is interesting to note that Eq. (4) is similar to the one obtained by Bradley *et al.*[4,5] for the thermoelectric power of liquid metals. In their expression, U^2 is the average of the square of the matrix element over all configurations of atoms in the liquid, and S is the experimental structure factor. The success of the pseudopotential method as used by Giaever[6] and by the authors[3] in the study of order dependence of resistivity of Cu_3Au suggests its applicability to the study of diffusion thermoelectric power of the same alloy above the critical temperature (390 °C). In this calculation, as in the previous investigation,[3] the form factors calculated by Animalu[7] are used (see Fig. 1) and the short-range order parameters measured by Moss are used for calculating the structure factors.

The structure factors for $T = 405$ °C and $T = 460$ °C are shown in Fig. 2. We found that as T increases from 405 to 460 °C the diffusion thermoelectric power decreases from 2.09 to 2.05 μV/deg. In the case of complete disorder, we found $Q_D = 191$. Thus, our theoretical calculations show that $dQ_D/d\delta$, where δ is the short-range order, is positive.

Airoldi *et al.*[8] studied the thermoelectric power of Cu_3Au as a function of order. However, their measurements are in the temperature range 18–1000 °K in which the phonon drag effects must also play an important role in the behavior of thermoelectric power. Since the separate contributions due to order and to phonon drag are very difficult to assess, a meaningful comparison between our calculations and the experimental results cannot be made. We hope that this paper will stimulate further experimental investigations such as measurements on the quenched pure sample at low temperatures (i.e., well below 10 °K) where the lattice vibrations are quenched and the effect of order becomes dominant.

We are grateful to Dr. A. O. E. Animalu for sending us the form factors of the noble metals.

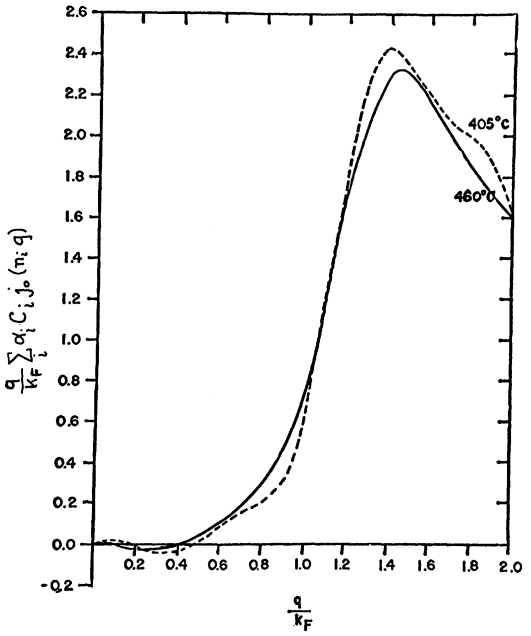

FIG. 2. Structure factor of Cu_3Au as a function of q/k_F at $T = 405$ °C and $T = 460$ °C. The calculation is based on Moss's measurements.

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On High-Electric-Field Conductivity in n-Type Silicon†

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The theoretical results of Basu and Nag on the high-field mobility of electrons in Si for any arbitrary direction of field are discussed, taking into account the intervalley electron-phonon scattering mechanisms. An up-to-date picture of these scattering mechanisms is outlined and shown to fit satisfactorily the electron drift velocity between 77 and 300 °K, from the Ohmic up to the saturation region. Nag, Paria, and Basu's (NPB) ratio of cool-to-hot valley population for electric fields along the ⟨100⟩ direction is also successfully interpreted.

In a recent paper, Basu and Nag[1] (hereafter referred as BN) have derived theoretical expressions for the high-electric-field mobility of carriers in n-type Si, for any arbitrary direction of field. They have also criticized the lattice-scattering picture used by Costato and Scavo (CS).[2,3]

We wish to show here that excellent agreement between experimental and theoretical findings on high-field electron drift velocity in Si can be obtained making use of Dumke's[4] model in place of Long's[5] model for intervalley scattering mechanisms, that the theoretical expressions of BN are inconsistent with the intervalley scattering mechanisms they assumed, and that BN erroneously interpreted the approach of CS.

The theoretical approach of BN can be summarized as follows: They assumed a carrier concentration for which the symmetric part f_0 of the distribution function is Maxwellian. Making use of the intervalley phonon energies of Long,[5] and taking into account lattice scattering only, they obtained results on hot-carrier mobility not in good agreement with the experimental findings of Nag, Paria, and Basu[6] (NPB), and found the ratio of cool-to-hot valley population (n_c/n_h) in sharp disagreement with the values obtained from the analysis of experimental results of NPB. BN believe their discrepancies arose because of a large effect of intervalley scattering in the energy and momentum exchange processes.

We would like to comment on the theoretical procedure used by BN and to show how results of NPB on n_c/n_h may be satisfactorily interpreted by means of our theoretical approach.[7,8]

BN used for the intervalley electron-phonon scattering mechanisms the phonon energies assumed by Long,[5] i.e., the f-type and g-type scattering mechanisms are caused by interaction with phonons with an equivalent temperature of $\theta_f = 630$ °K, and of $\theta_g = 190$ °K, respectively. Long[5] pointed out that these energies were obtained through an average and were not necessarily to be considered as "true values for real phonons."[5] The ratio of f-type to g-type coupling constants was taken by BN to be $W_1/W_2 = 3.3$, thus, with an enhanced predominance of f-type over g-type scattering. To solve the problem for the asymmetric part f_1 of the distribution function for any arbitrary direction of the applied electric field, they used the transformation of Herring Vogt.[9] However, let us point out that the above transformation cannot be applied to many-valley semiconductors, if it is not possible to treat the valleys as independent of each other, as was inferred by Asche and Sarbei.[10] Consequently, since BN assumed f-type scattering to predominate over g-type scattering, their procedure in using Herring and Vogt's[9] transformation is inconsistent. However, the results of BN can be thought of as an approximation to the problem, since it may be assumed that "the collision terms are given in the same form as if there would be spherical surfaces of constant energy, and in the