with decreasing lattice parameter. Apparently in the superconducting high-pressure phase the bound-state character of the $4f$ electron at zero pressure (which gives rise to antiferromagnetism in the β phase) is completely removed. From the results the fascinating question again arises whether the nonmagnetic "collapsed" α phase of very high-purity cerium will become superconducting also at a certain pressure. Experiments down to 0.3°K will be done in the near future. Furthermore, a determination of the structure of the superconducting high-pressure phase will be helpful for an understanding with regard to the superconductivity of thorium.

I would like to thank Professor B. T. Matthias and T. F. Smith for their encouragement and continuous interest. Collaboration with A. Eichler in building the equipment is greatly appreciated. The lot of pure cerium which showed superconductivity was kindly supplied by E. Corenzwit of the Bell Telephone Laboratories, Murray Hill.

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NEW MODEL FOR INTERFACE CHARGE-CARRIER MOBILITY: THE ROLE OF MISFIT DISLOCATIONS

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It is suggested that consideration of misfit dislocations is essential for analysis of mobility in metal-oxide-semiconductor inversion layers. Occurrence of such dislocations is generally expected for interfaces. Also, aspects of "surface" state behavior fit well with the dislocation model.

Study of inversion layers at the $Si-SiO_2$ interface over the past several years has provided extensive experimental information on carrier mobilities in such layers.[1-6] However, a satisfactory theoretical understanding of these data is still lacking. Early interpretations were generally based on the assumption of diffuse or partially diffuse surface scattering, but deficiencies of this theory have already been pointed out.[3,4,7] As an alternative, scattering by surface charges has recently been proposed in a number of papers, both in nonquantum[4,8] and also in quantum[9] formulations. However, this approach also presents difficulties: (1) One of the nonquantum approaches[8] assumes the surface charge to be localized strictly at the surface, and concludes that the resultant mobility will always be equal to or higher than that resulting from completely diffuse scattering; experimentally, at least some mobility values are lower.[10] (2) The other nonquantum approach[4] gives better agreement with the data, but assumes a conversion of surface charge into equivalent volume charge; this is arbitrary, and moreover implies "surface" charge extending up to ~300 Å into the material. (3) As to the quantum formulation, no agreement is obtained between the theoretical[9] and the experimental[6] variation of mobility with gate bias.

In the present paper, we propose that so-called misfit or interfacial dislocations fulfill a crucial role in determining interface properties in general, and mobility behavior in particular. In fact, consideration of such dislocations for interface properties appears not only reasonable but essential: Their occurrence is expected on energetic grounds in cases of lattice mismatch,[11] and moreover, they have been observed even in systems with much less lattice mismatch than Si-

SiO_2, for instance,[12] GaAs-Ge. As will be shown, the misfit-dislocation hypothesis can qualitatively account for several heretofore puzzling aspects of mobility behavior. For quantitative agreement, inclusion of quantum effects appears required; for instance, combination of the two effects leads to a very reasonable fit to data of Arnold and Abowitz.[4] Detailed considerations will be limited to the n-channel case in the present paper, but the overall model should apply equally well to the p-channel case.

The proposed structure for the dislocations is that of a two-dimensional network of lines or long rods located in the plane of the interface,[13] as is observed[12] for GaAs-Ge. It will be assumed that the experimentally observed "surface" states which act as carrier traps[14] at the Si-SiO_2 interface are not randomly distributed, but are states of the misfit dislocations and thus bunched along the dislocation lines. It follows from the model that the observed density of "surface" states is equal to the product of the density of the dislocations times the number of states per dislocation. It is also assumed that the energy-level structure of these states is as discussed in Ref. 4: States in the upper half of the energy gap are of the acceptor type, and thus charged when occupied by electrons, with the states below mid-gap of donor type. With this assumed acceptor-donor behavior, the dislocations are charged in inversion, resulting in a mechanism for mobility reduction entirely analogous to that given for bulk dislocations[15]: Free charge is repelled, and a cylinder (or hemicylinder, for the present surface case) of very poor conductivity forms around each dislocation; this results in a shift of the current lines and a reduction in effective mobility.[15] However, there is a crucial quantitative difference with the bulk case: If the hemicylinder of charge repulsion extends downward through the entire inversion region (or "channel"), the dislocations act as insurmountable walls to current flow and the resultant mobility reduction will be much larger than would occur with bulk dislocations. Similarly, the effect is also larger than that resulting from randomly distributed surface charge (as in the Greene-O'Donnell[8] theory). Moreover, estimates based on results of Stern and Howard[9] show the channel to be very narrow [≈30-40 Å for the (100) surface and ≈120-160 Å for the (111) surface], so that blockage through the full depth appears very likely.

The observed conductivity σ can be represented as

$$\sigma = e\bar{n}\mu_{\text{eff}}, \tag{1}$$

where μ_{eff} is the effective (observed) mobility and e is the electronic charge. The quantity $\bar{n}$ is the total mobile-carrier concentration; it is given by

$$\bar{n} \approx n_0 + 2d_t n_t, \tag{2}$$

where n_0 is the concentration of free carriers, n_t that of carriers trapped on the dislocations, $2d_t$ is the area density of the dislocations, and where the condition $2d_t \ll 1$ has been assumed. Denoting mobility and conductivity of the Si in the absence of dislocations by μ_0 and σ_0, respectively, one thus obtains

$$\mu_{\text{eff}}/\mu_0 = (\sigma/\sigma_0)[n_0/(n_0 + 2d_t n_t)]. \tag{3a}$$

Note that for $n_0 \gg 2d_t n_t$,

$$\mu_{\text{eff}}/\mu_0 = \sigma/\sigma_0. \tag{3b}$$

Assuming blockage of the entire channel, the calculation of σ/σ_0 is a two-dimensional problem. Moreover, a model of long thin ellipses for the dislocation rods results in easy evaluation of σ/σ_0 by a treatment analogous to that given for example by Sillars[16] for the dielectric properties of dispersed ellipsoids. It will be assumed that the ellipses are randomly distributed spatially. Their orientation will be taken such that half are parallel and half are perpendicular to the applied field; some regularity in orientation of dislocations is expected on crystallographic grounds, and the parallel-perpendicular arrangement should be representative. The current blockage by the parallel ellipses can be shown to be negligible and that for the perpendicular ones is approximately (for $\delta \ll 1, d_t \ll 1$) given by

$$\frac{\sigma}{\sigma} = \frac{1}{1 + d_t/(\delta + \sigma_t/\sigma_0)}, \tag{4}$$

where d_t is the area density of the perpendicular dislocations, σ_t is their conductivity, and $\delta = 1 - l_a/4\pi$, with l_a the two-dimensional analog of an integral defined by Sillars.[16] By evaluation of l_a one obtains

$$\delta = 1 - (1 + a/b)^{-1}, \tag{5}$$

where a and b are the axes of the ellipses, the a axis being parallel to the field.

A comparison of the theory with experiment can be obtained by use of data[4] of mobility versus filled surface states, with d_t taken proportional to the density of these states, and with the assumption that $(\delta+\sigma_t/\sigma_0)$ is the same for all samples. This comparison can readily be carried out under the condition $n_0 \gg 2d_t n_t$, which is very likely valid in the range in which the data were taken. The result is shown in Fig. 1, with μ_0 taken as the bulk drift mobility (=1350 cm^2/V sec)[17]; the agreement can be seen to be comparable, and perhaps slightly better, with that given by the Arnold-Abowitz[4] theory.

Recent work[6,9] has emphasized the probable importance of quantum effects; so a test of the model with inclusion of such effects seemed desirable. As discussed by Fang and Fowler[6] the (111) surface is expected to have almost all electrons in the ground state even at room temperature. For comparison with the present model, one requires an estimate of the resultant reduction of lattice mobility. This was obtained by use of equations given by Tavger and Demikhovskii[18]:

$$\mu=\frac{e}{m^*}\int_0^\infty \tau(y) y e^{-y} dy, \tag{6a}$$

$$y=\hbar^2k^2/2m^*k_0T, \tag{6b}$$

$$\tau=L\hbar^3\rho c_l^{\,2}/3m^*E_1^{\,2}k_0T, \tag{6c}$$

where L is the (inversion) layer thickness, k_0 is the Boltzmann constant, and the other symbols have the usual meaning. In the present evaluation, the conductivity effective mass was used in Eq. (6a), and the density-of-states mass in Eq. (6c), with both obtained as appropriate for the (111) surface from the results given in Stern and Howard,[9] Table I. The channel width (L) for the Si (111) surface is estimated at 120-160 Å [with this value obtained from Stern and Howard[9] Eqs. (22) and (42), with the appropriate effective mass from their Table I]. Use of the lower value shows that the resultant (111) mobility can be reduced as much as a factor of 0.6 compared with the bulk mobility. As to the (100) surface, Fang and Fowler[6] estimate that the effects of quantization may be negligible by room temperature. We will consequently assume the mobility along this surface to be equal to the bulk drift mobility. Figure 2 shows the resultant fit to the data of Ref. 4, again taking d_t proportional to the density of surface states and assuming $[\delta+\sigma_t/\sigma_0]$ to be the same for all samples; the value of μ_0 for the (111) surface was taken as 880 cm^2/V sec, i.e., 0.65 the bulk value, with the assumed reduction thus being slightly less than that estimated above as the maximum likely. The match to the (111) points is good (as it also is in Fig. 1), and is improved over that of Fig. 1 for the (100) points; over all, the agreement is quite satisfactory.

A further test of the present model is by comparison with mobility variation with gate bias (i.e., with degree of inversion), where a maximum has been observed[6] in the region near pinch-off. Analysis of Eqs. (3a) and (4) shows

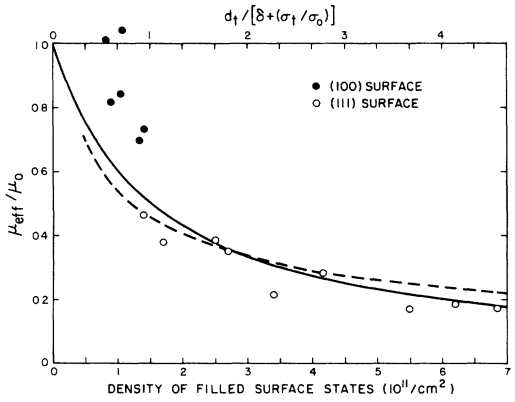

FIG. 1. A plot of the ratio of effective mobility (μ_{eff}) to mobility in the absence of dislocations (μ_0) against surface-state density and against the theoretical quantity $d_t/(\delta+\sigma_t/\sigma_0)$ given in Eq. (4). For the data points, which are referred to the lower scale, μ_{eff} and the density of states are from Ref. 4, and μ_0 was taken as 1350 cm^2/V sec. The solid line is theoretical, based on Eqs. (3b) and (4), and is referred to the upper scale. The dashed line is the theoretical curve of Ref. 4 and is referred to the lower scale.

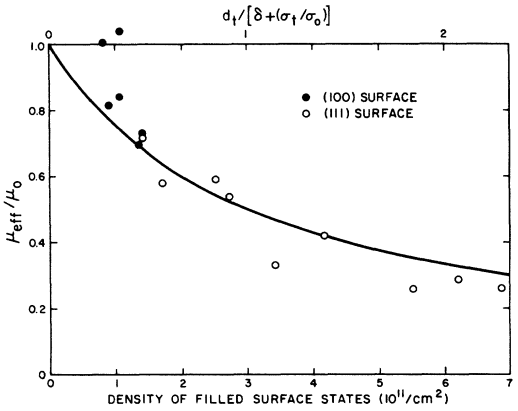

FIG. 2. Same as Fig. 1 (with the omission of the dashed curve) except that a quantum correction has been applied to the mobility of the (111) surface, with μ_0 for this surface consequently taken as 880 cm^2/V sec.

the theoretical curve to give a maximum as a function of n_0/n_t; since n_0/n_t is an increasing function[19] of bias, a maximum with bias also results. Moreover, the maximum would generally be expected to be at a low value of n_0, i.e., close to pinch-off [specifically, at $n_0/n_t \approx (2\beta)^{1/2}$, where β is the ratio of mobility in the dislocation region to μ_0]. Consequently, agreement in this respect is also very satisfactory.

The observed decrease of mobility with substrate doping[6] can also be understood on the basis of the present model, since doping decreases the bulk mobility (μ_0) via ionized-impurity scattering.

Finally, it is worth noting that the presence of misfit dislocations can also account for a number of results on Si-SiO_2 "surface" state behavior: (1) A higher density of surface states is generally observed on the (111) surface than on the (100) surface.[4,20] As pointed out for instance by Jaccodine and Schlegel,[21] there is greater lattice mismatch at the SiO_2-(111)Si interface than at the SiO_2-(100)Si interface. Thus, assuming the dislocation density to increase with mismatch, the observed orientation dependence of the density "surface" states follows as an obvious consequence of the degree of mismatch. (2) The postulated acceptor-donor behavior[4,22] correlates very well with the recent observation[23] of analogous behavior of dislocations in bulk Si. (3) A considerable amount of evidence indicates that the surface states mostly form a continuum of levels in the energy gap.[6,22,24] In addition, it has been shown that formation of an impurity-type conduction band by the surface states can satisfactorily account for $1/f$ noise in metal-oxide-semiconductor devices.[25] With a spatial density of 10^{11} states/cm^2, which is a commonly observed value, randomly spaced imperfections would be $\approx$300 Å apart; judging by the bulk situation[26] such a separation should result in little or no energy spread of these levels, and certainly no banding. However, for dislocations band formation is theoretically predicted,[27] with some experimental evidence for this effect also available.[28] Again, the misfit-dislocation model correlates very well with the observations.

In conclusion, it has been shown that a wide range of Si-SiO_2 interface data can be qualitatively explained by a misfit-dislocation model. Quantitative agreement, where tested, appears quite satisfactory with inclusion of quantum effects. Further quantitative analysis of the model is in progress.

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STRUCTURAL PHASE TRANSITIONS IN PEROVSKITE-TYPE CRYSTALS

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We introduce a simple model Hamiltonian for the study of phase transitions in perovskite compounds ABO_3 involving rotations of BO_6 octahedra. Depending on the relative magnitude of the anharmonic coefficients, we find a transition to the tetragonal or to the trigonal phase. We obtain the temperature dependence of the rotation angle below the transition temperature T_a, and of the soft-mode frequencies associated with the transition both above and below T_a. The coupling to an elastic deformation field is briefly discussed.

Recently, considerable experimental progress has been made towards the understanding of purely structural second-order phase transitions occurring in crystals of the perovskite family ABO_3. This concerns structural analysis using EPR methods,[1] Raman scattering,[2] and neutron diffraction.[3] The EPR results demonstrated the essential static characteristic of the transition, which is peculiar to the perovskite structure: The BO_6 octahedra rotate about a tetragonal axis in $SrTiO_3$ and about a trigonal axis in $LaAlO_3$, and it was found that the normalized rotation angles vary quantitatively in the same way as a function of reduced temperature below the transition.[1] It was concluded that the rotation angle is the order parameter for this type of transition. Associated with the transition, one expects the occurrence of soft modes[4,5]: The frequencies of those normal modes, which transform like the order parameter, should become zero at the transition temperature T_a. For the case considered, this is the triply degenerate mode at the R corner of the Brillouin zone transforming like the axial vector representation Γ_{15}' if the origin is chosen at the B atom. This choice of origin is more appropriate to the present case than that used by Cowley,[4,6] for which the representation is Γ_{25}. Such a soft mode has recently been observed in neutron diffraction by Shirane[3] in the high-symmetry phase of $SrTiO_3$. Due to the symmetry breaking at the phase transition, the mode is split below T_a into two branches situated at the zone center and transforming like Γ_1. Both branches are then Raman active and have been seen by Fleury, Scott, and Worlock.[2]

In this note, we study in a simple model the nature of the transition, the behavior of the order parameter, and the dynamics of the soft modes above and below T_a. We consider only the triply degenerate Γ_{15} R-corner mode, and neglect the motion of all other degrees of freedom. This mode can be built up from localized displacement fields $\vec{R}(l)$ associated with each cell (cell index l), in much the same way as the electron wave functions of a given band can be built up from localized Wannier functions. The experimental results suggest that these $\vec{R}(l)$ are essentially rotations of BO_6 octahedra about the cell center, with smaller displacements of more distant oxygen atoms (Fig. 1). The three independent rotations about the cube axes permit the

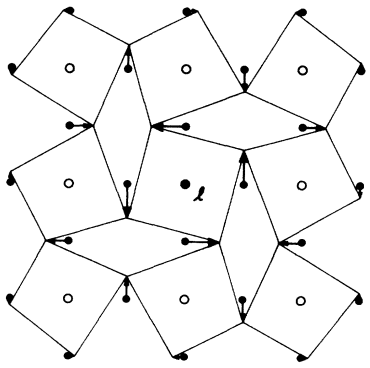

FIG. 1. Displacement field of the Wannier-type function $\vec{R}(l)$.