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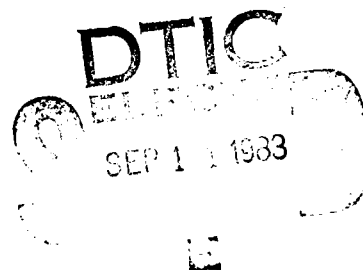
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FOURTH EUROPHYSICAL CONFERENCE ON LATTICE DEFECTS IN IONIC CRYSTALS
L. SLIFKIN Univ. of North Carolina
26 JUNE 1983

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This report discusses conference papers that dealt with ionic defects, such as vacancies, solute ions, and dislocations.

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FOURTH EUROPHYSICAL CONFERENCE ON LATTICE DEFECTS IN IONIC CRYSTALS

The fourth Europhysical conference dealing with the properties of defects in ionic crystals was held at Trinity College, Dublin, from 30 August through 3 September 1982. Previous meetings in the series were at Canterbury (1979), Berlin (1976), and Marseille (1973).

The conference papers were in two reasonably distinct groups: (1) color centers and spectroscopy of solute ions, and (2) ionic defects, such as vacancies, solute ions, and dislocations. Apart from brief mentions of plenary lectures, this report focuses on sessions dealing with the ionic defects and does not discuss the contributed papers dealing with color centers and related topics. The complete set of papers is to appear in a special issue of the journal *Radiation Effects*.

The first plenary lecture, presented by R. Macfarlane (IBM–San Jose) was a discussion of modern techniques for high resolution optical spectroscopy of defects in crystals. In particular, Macfarlane described the use of laser light to "burn" a narrow spectral hole in the inhomogeneously broadened zero-phonon line of a color center or a rare-earth impurity, thereby making possible investigations such as Stark effect spectroscopy. Another type of high-resolution spectroscopy, based on electron paramagnetic resonance (EPR), was reviewed by J. Niklas (Paderborn). He showed how the complicated spectra of systems with several types of low-symmetry defects could be resolved and refined by a combination of computer processing and multiple resonance techniques.

In another plenary lecture, J. Langer (Polish Academy, Warsaw) surveyed the effects of coupling between the phonons and the electronic system of a defect. He treated the processes of self-trapping and solute-trapping of a photocarrier and showed how an energy barrier can come about. He also discussed the role of phonons in recombination (radiative versus nonradiative de-excitation) and the resulting effects on defect reactions and on defect migration. A. Stoneham (Harwell) and M. Sangster (Reading) presented Harwell automatic defect evaluation system (HADES) calculations of the so-called "negative-U" centers—i.e., centers with one charge state that is unstable in the crystal relative to a disproportionation. Stoneham pointed out that the main factor in determining negative U is the polarization of the lattice and that one can do more accurate calculations of this on ionic crystals than for semiconductors. He then gave results of some calculations on solute centers in alkali halides and several oxides.

Several papers dealt with the trapping of photocarriers in the silver halides, studied largely by EPR methods. F. Granzer and Th. Müssig (Frankfurt) reported measurements on irradiated crystals of the mixed NaCl/AgCl system. In the NaCl-rich regime, the Ag^+ ion acts as an electron trap, forming Ag°. With increasing AgCl content, however, the Ag° center becomes increasingly unstable, and a new center, Ag^{2+}, appears. Thus, it seems that the Ag^+ can function either as an electron trap or a hole trap, depending on the ratio of NaCl to AgCl concentrations. During the discussion of the paper, M. Olm (Eastman Kodak, but presently on leave at Leicester) described similar experiments which she has been performing and which essentially verify the results. Two other points of interest: (1) in the two-phase region, irradiation induces a new, sharp line that appears to be due to conduction electrons in the boundary regions (as previously seen in another context by Eachus and Graves of Kodak), and (2) the line shape of the signal from the electrons appears to depend on the size of the overall sample, as though the electrons "see" the entire specimen. In another paper, Olm and R. Eachus described

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experiments on the trapping of photo-electrons in AgCl and AgBr doped with Os^{3+}. For complete charge compensation, the Os^{3+} would have to be associated with two cation vacancies, and the EPR experiments indicate that such is always the case, even when the solute has captured an electron to become the divalent ion and has been warmed to room temperature. A related system, $AgBr:Ir^{3+}$, was discussed by J. Spoonhower (Kodak). He has studied the excitation spectrum and the phonon structure of the luminescence, as well as the EPR spectrum of photo-produced Ir^{2+}, and concluded that at least two species of solute--as yet unidentified--must be involved. J. Hamilton (Kodak) considered the relative cross sections for capture of electrons and holes by the growing sublatent image in silver halides, and concluded from photographic evidence that the two cross sections are about the same, suggesting that the latent image site is a kink whose charge is one-half the electronic charge. The process of self-trapping of the photohole at low temperatures in AgCl was discussed by E. Laredo (Simon Bolivar Univ., Caracas) and a group from the Univ. of North Carolina; they have demonstrated the existence of a predicted energy barrier, 1.7 meV, and have obtained binding energies and bandwidths from the migration kinetics.

Several papers dealt with ion transport phenomena. The effect of a temperature gradient on the migration of defects was analyzed by M. Gillan (Harwell) in terms of an atomistic treatment of thermopower and the heat of transport of defects, and as functions of doping and the electrode properties. The calculations give heats of transport for the various defects in simple halides that are negative and slightly larger than the migration activation energies--in substantial agreement with the little experimental data currently available. B. Zeqiri and A. Chadwick (Kent) re-ported a recent experiment on thermopower in pure and doped $SrCl_2$; the researchers took steps to assure reversibility at the electrodes. The experiment essentially agreed with Gillian's calculations for the anion vacancy, but was in both qualitative and quantitative disagreement in the case of the interstitial. A more general, phenomenological treatment of defect migration in the presence of a force field was given by G. Murch (Argonne), with special emphasis on large concentrations of defects. Partial blocking at electrodes affects ionic conductance. A. Kessler and W. Appel (Stuttgart) showed that the effects can be used to determine bulk conductivity. A measurement of the time-dependent thermally stimulated current yields a result that does not depend on knowledge of the extent of electrode blocking.

An experimental paper by A. Laskar and P. Cardegna (Clemson) and a theoretical one by J. Corish, N. Bannon (Univ. College Dublin), and P. Jacobs (Univ. Western Ontario) addressed the question of the nonlinear Arrhenius plots for ionic conductivity and tracer diffusion in the silver halides. If the only effect were a temperature dependence of the defect enthalpies and entropies, all curvatures should be of the same magnitude. However, oversized cations show no detectable deviation from an Arrhenius relation, and this was discussed in terms of a compensating temperature dependence in the solute ion's jump energy, with perhaps a small contribution from the association energy. Similarly, a HADES calculation of defect parameters in KCl by I. Hooton and P. Jacobs (Univ. of Western Ontario) gave results that fitted experimental parameters satisfactorily. In contrast, J. Dryden and J. Cook (CSIRO, Lindfield, Australia) reported on measurements (by thermally stimulated depolarization) of the kinetics of association between the anion vacancy in alkali halides and added S^{2-} or O^{2-}. Dryden and Cook said that values of the migration

energy from the anion vacancy agreed with earlier results from conductivity but were higher than those obtained from HADES calculations by at least 50%. The values range from 1.05 to 1.23 eV and greatly exceed the 0.7 eV usually accepted. No explanation for the discrepancy is yet available. An NMR study of ion migration in pure and doped LiI, by K. Budde (Bochum), resulted in a determination of the Schottky formation energy (1.28 eV) and the cation vacancy migration energy (0.36 eV), and demonstrated that addition of Cu^+ increased the concentration of cation vacancies. It appears that the cuprous ion is interstitial, perhaps because of the large polarizability of the neighboring iodide ions.

One might ask quite a different question about ionic transport: what happens to vacancy concentrations and mobilities in solid solution mixed crystals? One such system, KI/RbI, has been studied by L. Bonpunt (Bordeaux), F. Beniere (Rennes) et al. The researchers measured the ionic conductivity and the diffusivities of all three tracers over the entire range of composition. They find that the vacancy concentration goes through a maximum near the 50/50 composition, as do the tracer diffusivities, but not the conductivity (apparently because of a significant number of vacancy pairs at mid-composition). A study of divalently doped TlCl was reported by J. Quigley (Trinity College, Dublin) J. Corish (Univ. College Dublin) et al. By extending the conductivity measurements to rather low temperatures with the technique of thermal depolarization, they were able to see the hitherto unobserved extrinsic region in the material. HADES calculations of point defect properties in TlCl agreed with the experimental results.

R. Capelletti (Parma) reviewed the clustering of solute-vacancy complexes, emphasizing the wide range of techniques used both to measure and to analyze aggregation, precipitation, and dissolution. She described not only the successes in the field (i.e., the elucidation of the originally "anomalous" third-order kinetics for loss of solute-vacancy complexes), but also the difficulties and some remaining puzzles. Further, detailed examples of this sort of research were described by Capelletti et al., who have used thermally stimulated depolarization to study nucleation and growth of a second phase in heavily doped NaCl:Pb; by Agullo-Lopez, Sole, and Zaldo (Autonomous Univ., Madrid), who used Pb^{2+} traces as an optically sensitive probe to study the precipitation process in NaCl:Ca; and by M. Moreno and F. Rodriguez (Santander, Spain) and Andres et al. (Autonomous Univ., Madrid), who monitored the formation of the Suzuki phase in NaCl:Mn by EPR and several optical techniques. Finally, a somewhat different type of phase separation, the formation of colloidal metal particles in irradiated insulating crystals, was reviewed by A. Hughes (Harwell). Although the effect is seen in a wide variety of materials, the best-known example (other than the photographic process in AgX) is the aggregation of F-centers in irradiated alkali halides. The efficiency of colloid formation is a nonmonotonic function of temperature and depends sensitively on dose rate and dislocation density. Hughes showed that a model worked out by Jain and Lidiard is in qualitative agreement with many features of the phenomenon, but that a number of perplexing questions remain.

A paper by E. Duval, M. Barland, and A. Nouilhat (Lyon) described a series of experiments on the effects of an electric field on the thermoluminescence of X-irradiated $KI:Eu^{2+}$, from which they could deduce information about the hopping of trapped electrons from one Eu site to another. The results are consistent with a model in which the crystals contain a Eu-rich phase or domains, with a spacing of 28 angstroms between Eu ions, independent of the previous cooling rate. LiF:Ti (and LiF:Ti, Mg)

is another material in which the luminescent properties are important—for dosimetry, in this case; I. Foldvari et al. (Hungarian Acad. Sci.) did the study. They described an experiment on the effects of annealing atmosphere on the ionic conductivity, optical absorption, and EPR, both before and after X-irradiation. They found that the Ti is present as Ti^{3+} in an inert growth atmosphere, and as Ti^{4+} in air, and that the local coordination of the Ti ions is strongly influenced by the presence of any Mg.

In the past there have been a few observations of an enhancement of ion mobility by electron excitation, but little is known about the phenomenon. Two further examples were given at the conference. L. Delgado (Junta de Energia Nuclear, Madrid) has found that X-irradiation of KCl:Cu stimulates the aggregation of the solute, as manifested through changes in photoluminescence. Similarly, M. Aguilar et al. (U. Autonoma, Mexico) showed an irradiation-stimulated aggregation and precipitation in alkali halides doped with Eu^{2+}, as monitored by EPR, optical absorption, and luminescence. Even when the solute is aggregated into metastable clusters, X-irradiation causes conversion into a more stable precipitate phase.

Several papers dealt with materials of the type MX_2, especially those with the fluorite structure. V. Sahni and P. Jacobs (Univ. of Western Ontario) described calculations of the entropy and volume of formation of anion Frenkel defects in CaF_2, in a quasi-harmonic approximation, and with a periodic boundary condition on the "specimen." Their formation volume results agree with experiments, and their formation entropies were found to increase strongly with the increase in lattice parameter that occurs at higher temperatures. The complexes formed between trivalent cations and interstitial fluorides were studied in $SrF_2:La^{3+}$, in research done by N. Suarez, E. Laredo, D. Figueroa, and M. Puma (U. Simon Bolivar, Caracas). By monitoring thermally stimulated depolarization peaks as a function of dopant concentration and temperature, the workers were able to identify one peak due to $La^{3+}F_i^-$ and two peaks due to configurations of $La^{3+}(F_i^-)_2$; note that the latter complex is overcompensated. More complicated clusters were investigated by J. Corish (Univ. College Dublin), A. Chadwick (Kent), and C.R. Catlow (Univ. College London), who obtained single-crystal neutron diffraction patterns from CaF_2 highly doped with La^{3+} or with the smaller Er^{3+}. They could identify several geometries of cluster, including some with an overcompensation of F_i^-. A similar material, PbF_2, was studied by M. Wintersgill et al. (US Naval Academy and Kent); they followed the dielectric relaxations of complexes produced by doping with a series of trivalent rare earths and saw peaks attributable to simple complexes and to a variety of clusters. When the dopant radius was small, a great many peaks (in some cases at least nine) could be resolved, quite unlike the case of the alkaline earth halides.

The fluorite materials are especially interesting at temperatures approaching the melting point, where they exhibit the high ionic conductivity characteristic of solid electrolytes. Many questions have arisen in connection with the numbers of Frenkel defects in the regime, the relative contributions to ion transport from interstitial fluorides and anion vacancies, and the effects of dopants. The questions were reviewed by A. Chadwick (Kent), who pointed out that much of the older data is perturbed by contaminant (H_2O and O_2), that the concentration of defects in the high-tempera-

ture range is only about 2 to 3% instead of the much higher values formerly accepted, that the anion sublattice is not liquid-like, and that clusters (e.g., the so-called 2:2:2 cluster) can explain many of the anomalies. During the discussion that followed, however, arguments were presented against the significance of the clusters in accounting for the defect properties. A more detailed picture of the dynamics of the anion vacancy migration in $SrCl_2$ emerged from the incoherent neutron scattering results reported by P. Schnabel et al. (Oxford, Harwell, Hahn-Meitner Inst., and Inst. Laue-Langevin). They determined residence and jump times and the jump directions.

An interesting result for the quite different material MgF_2 was presented by A. Norwick and J. Toulouse (Columbia), who studied the effect of doping with Li^+ on the ionic conductivity and the diffusivity of Mn^{2+} solute ions. It appears that the state of the Li^+ changes drastically with temperature: near room temperature it enters the MgF_2 as a Li_2^{++} pair; above about 300°C, the pairs begin to dissociate into self-compensated substitutional-interstitial defects; while above 800°C, the Li^+ exists predominantly as the interstitial. Another set of substances, the alkali sulfates, have a high-temperature transition to a "plastic" phase in which the sulfate ions rotate. This causes a high mobility of the alkali ions, by means of what A. Lunden, R. Aronsson, and L. Nilsson (Chalmers, Goteborg) call the "paddle-wheel" mechanism. In their most recent work, they measured the elastic constants and found that at high temperatures they are lower than those of ordinary ionic compounds by a factor of 10.

Research on the oxides is much more difficult than work on crystals of the halides. It is harder to obtain pure materials, to add controlled amounts of dopants, to be certain of stoichiometry, and to perform experiments on such refractory substances. Nevertheless, the oxides are extremely important, both scientifically and technologically. Thus, a substantial number of papers at the Dublin conference dealt with lattice defects in such materials. A review of one aspect of point defect structure in crystalline and amorphous oxides, the asymmetric relaxation of neighboring ions, was presented by W.B. Fowler (Lehigh). He discussed the dependence of the resulting savings in polarization energy on the size and the electronic state of the central ion, and showed how off-center ions and valence alternation pairs could arise. The effects of such relaxation on the properties of trapped photocarrier centers can be large and pervasive. M. Sangster and D. Rowell (Reading) described HADES calculations of the force constants around lattice defects, and especially for the case of the interstitial oxide ion in UO_2. They see large (50%) increases and long-range effects. Thus, the simple "adding spring" models are incorrect because of the large effects of polarization. V. Butler and B. Fender (Univ. College London) also have used the HADES package to calculate the distribution of defects in calcia-stabilized zirconia and conclude that isolated point defects are in equilibrium with microdomains of a second phase. The large effect of elastic, in addition to coulombic, interactions in the formation of defect clusters was demonstrated by HADES calculations on oxides and halides, descr... by J. Kilner (Imperial College) and C.R. Catlow (Univ. College London). Thus, the size of the solute ion exerts a major influence on the ionic conductivity.

In the case of oxides of transition metals, the cation often can exist in more than one valence state, so the deviations from stoichiometry can be varied over a large range by control of the partial pressure of oxygen. This

can produce a variety of point defects, small and large clusters, and planar defects called crystallographic shear planes. An electron diffraction-microscopy study of the phenomena in $Fe_{1-x}O$ was reported by L. Hobbs and C. Lebreton (MIT), who emphasized how the ordering of the defect clusters depends on temperature and on deviation from stoichiometry. Using the HADES code, A. Cormack, G.R. Catlow (Univ. College London) and P. Tasker (Harwell) calculated the interaction between crystallographic shear planes. In particular, their calculation simulated WO_3-type materials, and it revealed the great importance of including ionic relaxation and long-range interactions. The same problems were attacked in a different way by G. Boureau and J. Marucco (Orsay), who calculated how the thermodynamic parameters affect the interactions between isolated point defects and the crystallographic shear planes. L. Bursill (Univ. of Melbourne), M. Blanchin (Lyon), and D. Smith (Cambridge) investigated crystallographic shear planes in reduced rutile. Transmission electron microscopy shows a more complicated distribution of defects in reduced rutile; it was found that dislocations are effective in stimulating the formation of crystallographic shear planes.

A review of the mechanisms of ion diffusion in stoichiometric and non-stoichiometric oxides was given by C. Monty (Meudon-Bellevue). The following techniques are available for the studies: tracer diffusion, conductivity, creep, doping, variation of stoichiometry, and computer simulation. Many problems remain, e.g., the difficulty of obtaining an intrinsic behavior, the slow migration of the less mobile component, uncertainties about whether a component migrates by vacancies or interstitials, the complications due to complexing, and effects of electronic conductivity. A study of the mobility and the trapping of monovalent cations in quartz (which always contains some Al^{3+}—hence the presence of M^+ compensators) was described by J. Martin (Oklahoma State), who showed how one can electrically sweep out any given M^+ and replace it with a different mobile cation. Moreover, ionizing radiation enhances the mobility of H^+ in SiO_2 and frees alkali ions from Al^{3+} sites. Solute diffusion in Al_2O_3, both undoped and doped with homovalent cations, was studied by B. Lesage and A. Huntz (Orsay), and G. Petot-Ervas (Villetaneuse). They also explored the effects of oxygen partial pressure, and compared diffusivities with conductivity to deduce concentrations of defects. Petot-Ervas and B. Sossa also reported studies of $Co_{1-x}O$, in which the effects of oxygen pressure and of doping on the conductivity could be determined to obtain information on the diffusivities due to both singly and doubly charged cation vacancies. A paper by A. Dominguez-Rodriguez (Seville) and J. Castaing (Meudon-Bellevue) showed how creep experiments can be used to obtain information about the diffusion of the slow component, the minority species. Thus O^{2-} diffuses by an interstitial mechanism in Cu_2O, by both vacancies and interstitials in CoO, and by only a vacancy mechanism in NiO.

H.-J. Matzke (Karlsruhe) discussed diffusion of cations in UO_2. The material has the fluorite structure, and the cation is the slow component; diffusion was monitored by alpha-particle spectroscopy. A large, temperature-independent enhancement resulted from fission events; the effect is much too large to be explained by the displacement spike model and might be caused by gradients of temperature or pressure in the spike region. Alpha-Ta_2O_5, another oxide in which the anion is the more mobile species, can be stabilized at lower temperatures by

addition of scandia. The effects of oxygen pressure on the conductivity of the material were measured by A. McHale (National Bureau of Standards) and H. Tuller (Massachusetts Institute of Technology). They saw both ionic and electronic contributions and concluded that defect interactions were very large. R. McKee (Oak Ridge) analyzed diffusion in $Fe_{1-x}O$; he related the chemical and tracer diffusivities and the correlation factor to the deviation from stoichiometry. F. Beniere, J.-P. Louboutin, and J.-I. Franco (Rennes) measured the self-diffusion of radio-tracers of Na^+ in polycrystalline β''-alumina below room temperature. The sectioning was done at room temperature and therefore had to be performed very quickly; the blade of the microtome the researchers used was a large diamond crystal. Their value for the activation energy, 0.30 eV, agrees with that for the conductivity of poly-crystalline material but is larger than that previously found for diffusion at higher temperatures in single crystals. All the results point to a diffusion barrier at the grain boundaries.

There were considerably fewer papers on dislocations than on point defects at the Dublin meeting. In a review lecture, P. Veyssiere (Poitiers) discussed how the dislocation core is affected by changes in composition and stoichiometry in oxides, along with resulting changes in climb dissocia-tion, stacking fault structure, space charge clouds, and dislocation mobil-ity. He considered diffusion-limited creep and showed how it can give infor-mation about the diffusivity of the slower component of the oxide. A related talk by A. Heuer (Case Western Reserve) emphasized the electron micro-scopy of dislocation loops in crystals such as Al_2O_3, for which the kine-tics of annealing can provide the best data on oxide diffusion yet available for sapphire. M. Blanchin, M. Vrinat, and A. Mebarek (Lyon) described plas-ticity and transmission electron micro-scopy experiments on slightly reduced rutile, for which the dislocation-point defect interaction is a determining factor.

Two papers dealt with pipe dif-fusion along dislocations. One, a computer simulation of MgO by J. Rabier and M. Puls (Poitiers), concluded that the large diffusivity along the core is due to a decrease in the vacancy forma-tion energy, not in the migration energy. The other, presented by P. Pratt and Y. Ho (Imperial College), was an experimental study of the disloca-tion tail in the low-temperature pene-tration profile of radiotracer sodium diffusing into very pure NaCl crystals. In the extrinsic region, the activation energy was 0.57 eV, compared with 1.25 eV in the bulk lattice.

The photoplastic effect (the effect of light on the flow stress) is interesting in alkali halide crystals containing F-centers: at low tempera-tures, F-light decreases flow stress and at higher temperatures increases it. T. Hagihara, Y. Inoue, and T. Okada (Osaka) correlated the transition temperature between the two regimes with that for the onset of photoconduc-tivity and were thereby able to explain the low-temperature effect in terms of a smaller elastic interaction between the dislocation and the F-center when the latter defect is in an electron-ically excited state. Above the transition temperature, the irradiation converts the neutral F-centers into charged F^- and F^+, which bind more strongly to the dislocations.

W. Robinson (DSIR, New Zealand) discussed the behavior of dislocation loops oscillating under a periodic stress. Robinson measured the damping, the dislocation displacement versus applied stress, and the piezoelectric effect of charged dislocations in NaCl crystals that had been bent to intro-duce an array of edge dislocations. The main question addressed in the work was the role of interaction between a charged dislocation and its space charge cloud. From the results, he concluded that while the line tension of the dislocation (not the electro-

static interaction) provides the restoring force, the damping is due primarily to the charge cloud, not phonons.

In another paper, Robinson and his colleagues discussed their measurement of the temperature dependence of the dislocation charge in KCl as a function of doping with Ca^{2+}. By determining the isoelectric temperature (where the charge density is zero) versus solute concentration, one can deduce the separate formation enthalpies and entropies of the two components of the Schottky pair. For example, the formation enthalpy is 1.24 eV for the cation vacancy and 1.34 eV for the anion vacancy.

Charged dislocations of KCl:Ca were also studied by T. Kataoka, L. Colombo, and J. Li (Rochester); they used two additional techniques: (1) a measurement of the minimum electrical field that will move the dislocations, and (2) a measurement of the potential difference produced across a specimen compressed between slightly tilted plates. In each case, the charge per unit length along the dislocation increases in magnitude with increasing calcium concentration and increasing temperature (in a range below room temperature). The results could be explained quantitatively in terms of the acquisition of cation vacancies by the dislocations. S. Racz, G. Turchanyi, and J. Janszky (Hungarian Acad. Sci.) studied the effect of charged dislocations on photocurrents in bent alkali halides containing F-centers. The observed photovoltages were discussed in terms of the fields due to the dislocations, but the results were rather complicated. N. Collins (Queen Elizabeth College) studied charged dislocations in AgCl and AgBr by monitoring the potential difference produced by a rapid indentation. The results were consistent with bursts of negatively charged dislocations moving away from the indenter, but a quantitative analysis was perturbed by the internal conduction of the crystal.

Only a few of the papers at Dublin dealt explicitly with free surfaces. L. Harris (Univ. of New South Wales) mounted a vibrating reed electrode above a cleaved (all in ultrahigh vacuum) crystal of NaCl and measured the variation with temperature of the surface potential. The sign of the charge (negative) and the value of the isoelectric temperature were the same as those found earlier for dislocations in the interior of the same material. Surface charges on silver halides were studied in two experiments reported by L. Slifkin, G. Farlow, A. Blose, B. Lounsberry, and J. Feldott (North Carolina). In one, the subsurface potential was mapped by the distribution of a radiotracer probe; in the other, the effects of such dipolar liquids as water and methanol on the jog densities were observed by means of changes in thin film conductance.

The energies of point defects on surfaces are unknown; in an attempt to remedy this, J. Kendrick, E. Colburn, and W. Mackrodt (ICI-Runcorn) used computer simulations. Compared to the bulk, a vacancy on the surface of MgO has smaller formation and migration energies but a stronger interaction with another vacancy. Calculations of the effects of surface ledges and kinks and of impurity ions are now under way. Other calculations of both surfaces and grain boundaries were reported by D. Wolf (Argonne). He concluded that a major factor in the cohesion of a boundary in an ionic crystal is the presence of various point defects, including segregated impurity ions.

The conference concluded with brief summary remarks by G.F. Imbusch (Galway). He commented on the following points: (1) the advances in our understanding of interactions between lattice defects, (2) the need to expand our computer codes so as to encompass more complex systems, (3) the growth in sophistication of methods to elucidate ion transport phenomena (including the demonstration of the reliability of the HADES computation), (4) the development

of very high time- and frequency-resolution in the study of color centers, and (5) the development of techniques that can single out a specific type of defect.

For this conference, as with the earlier meetings, the local organizing committee was supplemented by an international advisory group drawn largely, but not exclusively, from the scientific population of western Europe. In addition to the financial support provided by a number of Irish organizations, the European Research Office of the US Army and the US Office of Naval Research, London, offered assistance. The next in this series of conferences will be held in 1986 at the Univ. of Santander, Spain.

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