

14.2-8 NANODIFFRACTION AND SREM STUDIES OF SURFACES

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For crystals having flat faces more than 1000\AA in diameter or for bulk samples it is possible to obtain useful information on the surface structure by using a scanning transmission electron microscope in the reflection mode (SREM). In this way surface steps and other features have been seen with a resolution of 10\AA or better. The images may be correlated with local crystallographic information when the scan of the electron beam, diameter 10\AA , is stopped to obtain a diffraction pattern from any chosen picture element. Using these techniques studies have been made of the structure, epitaxial alignment and distribution along surface steps of 20\AA metal particles on oxide surfaces.

For crystals having flat faces $1\mu\text{m}$ or less in diameter information regarding surface structure and excitations can be obtained by directing an incident electron beam, 10\AA or less in diameter, parallel to the surface. The electron beam may be deflected by the potential field of the crystal extending into the vacuum and the nature of this field may be deduced from observations of the corresponding effects in the diffraction pattern. Strong diffraction effects may also be observed from the presence of a few atomic layers of a modified surface structure such as the reaction products of silver on MgO .

14.3-1 MOLECULAR ELECTRON-CORRELATION EFFECTS IN HIGH-ENERGY ELECTRON SCATTERING ON GASES. By M. Breitenstein, H. Meyer and A. Schweig, Fachbereich Physikalische Chemie, Universität Marburg, D-3550 Marburg, West-Germany.

Theoretical high-energy electron scattering studies are generally based on the first Born approximation and make use of approximated Hartree-Fock (AHF) molecular wavefunctions. In the case of total (elastic plus inelastic) scattering the calculated difference function between the molecular and independent atom model differential cross sections, $\Delta\sigma^{\text{tot}}(s)$, may differ significantly from the experimental results.

We have calculated $\Delta\sigma^{\text{tot}}(s)$ for some linear molecules (N_2 , CO , O_2 , F_2 , C_2H_2 , CO_2) using high-quality molecular AHF wavefunctions which were improved by extensive configuration interaction (leading to about 60% of the empirical electron correlation energy). The results obtained agree markedly better with the experimental data (as far as available) than those not including electron correlation. Still remaining discrepancies between theory and experiment may be overcome, to a large extent, by a simple procedure estimating the full electron correlation effect based on Tvard's theorem.

The correlation correction term of $\Delta\sigma^{\text{tot}}(s)$ turns out to be markedly affected by the elastic contribution which represents roughly one third of the total correction term. The correlation effect on $\Delta\sigma^{\text{tot}}(s)$ cannot be interpreted as a specific two-electron effect. Interestingly, in the case of N_2 the calculated total correlation energy is more affected by an increased electron attraction to the nuclei than by a diminished electron-electron repulsion, in contrast to the usual picture of electron-correlation effects. For more details see: M. Breitenstein, A. Endesfelder, H. Meyer, A. Schweig and W. Zittlau, Chem. Phys. Letters 97 (1983) 403.

14.3-2 THE MOLECULAR STRUCTURE OF THE METAL-METAL BOND IN THE GAS PHASE. By M. Fink and S. Ketkar, Center for Structural Studies, The University of Texas RLM 10.202 Austin, Texas 78712

The comparison of molecular structure parameters derived by diffraction from a solid and from the same compound in the gas phase gives a direct measure of the interaction of the neighbors on the free molecule in the crystal lattice. In most cases the changes in the bond lengths are small and only very detailed data can be used to gain further understanding about the intermolecular interaction. However, occasionally a case is found where the molecule alters its structure significantly when packed in a lattice. These compounds cause severe confusion in the studies of trends in sequences of related molecules. One example, in the family of metal-metal multiple bonds, is the Cr-Cr distance. The x-ray structure determination gives this distance as 21.6 nm while studies on triazines found a much shorter length of 19.8 nm . It was repeatedly stated that the interference of the axial Cr-Cr bond in $\text{Cr}_2(\text{O}_2\text{CCH}_3)_4$ was the major reason for the bond lengthening. Electron diffraction data were collected on $\text{Mo}_2(\text{O}_2\text{CCH}_3)_4$ and $\text{Cr}_2(\text{O}_2\text{CCH}_3)_4$ to determine the molecular structure parameters of the two compounds. The latter molecule presented a major challenge since it is very reactive and highly unstable at elevated temperatures. Our studies had to be performed at vapor pressures of a few millitorr. This was sufficient to record the differential cross sections and to use the data to determine the molecular structure parameters. These values can now be used in *ab initio* calculations in order to study the contributions of the 3d electrons to the multiple bond and to explain the photoelectron spectrum. The mean amplitudes of vibration give a first hint at the vibrational spectroscopy of this molecule.

14.4-1 HIGH RESOLUTION ELECTRON MICROSCOPY OF TOCHILINITE: A TERRESTRIAL ANALOGUE OF AN IMPORTANT EXTRATERRESTRIAL PHASE. By Michael E. Zolensky and Ian D.R. Mackinnon, SN4/NASA, Johnson Space Center, Houston, Texas, U.S.A. 77058.

Poorly characterized Fe-S-Ni-O phases (PCP's) may constitute up to 30% of some C2M carbonaceous chondrite matrices and are an important key to an understanding of solar evolution. On the basis of recent HREM studies of PCP's we have proposed that PCP's form at least two ordered, stable structures based upon alternating sequences of mackinawite- $[(\text{Fe,Ni})_9\text{S}_8]$ and brucite- $[\text{Mg}(\text{OH})_2]$ type layers (Nature, in press). These structures would have basal periodicities of 10.8\AA with a sub-cell repeat of 5.4\AA . This basal periodicity is precisely what is observed in PCP's. The terrestrial analogue of 10.8\AA PCP is tochilinite $[\text{6Fe}_{0.5}\text{S}\cdot 5(\text{Mg,Fe})(\text{OH})_2]$. Ion milled samples of acicular tochilinite from Cornwall, Pennsylvania, were examined with a JEOL 200CX electron microscope. High resolution images clearly reveal 5.36\AA sub-cell basal fringes, in good agreement with HREM images of one variety of PCP. An SEM study of Cornwall tochilinite revealed that the fibers consist of rolled sheets, in a manner analogous to chrysotile. This sheet curvature is caused by the structural misfit of the mackinawite and brucite layers. This layer misfit causes a high density of stacking faults along the layer planes, as revealed by HREM images. The degree of layer misfit is controlled by variations in the composition of each layer; eg. substitution of Ni or Mg into the mackinawite layer, and Al or Fe into the brucite layer. Compositional variations are frequently observed in a single tochilinite fiber. Additional complexity is caused by frequent cation vacancies within the mackinawite layer. Similar chemical variability and morphological features are also observed in PCP.