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SPRING COLLEGE IN CONDENSED MATTER ON QUANTUM PHASES
(3 May - 10 June 1994)

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BACKGROUND MATERIAL for lectures on

OPTICAL AND TRANSPORT STUDIES ACROSS THE METAL-INSULATOR TRANSITION

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These are preliminary lecture notes, intended only for distribution to participants.

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Optical and transport studies across the metal-insulator transition: A series of lectures for the Spring College in Condensed Matter on Quantum Phases Trieste, Italy 1994

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7 May: Can V_2O_3 be described by the Hubbard model?

An overview will be presented of different experimental and theoretical variables that can be used to approach the metal-insulator transition. The interesting case of V_2O_3 will be presented with emphasis on the fundamental parameters of the insulating state. A comparison will be made between new experiments and various approximate solutions of the Hubbard Hamiltonian. (See G. A. Thomas, et al., preprint.)

9 May: Comparison of disordered systems with theories of localization.

A comparison will be made between ideas about disordered systems and a classic example: Si:P. The optical excitation spectrum will be discussed over a wide range of impurity densities from isolated atoms to the metallic state. Open questions will be discussed. (See R. F. Milligan and G. A. Thomas, in "Annual Review of Physical Chemistry", S. Rabinovich, Ed., (Annual Reviews, Palo Alto, 1985); and T. F. Rosenbaum et al., Phys. Rev. B27, 7509 (1983).)

10 May: Impurity states and conducting states in high T_c oxides.

A comparison will be presented of the high-T_c oxides with both quasi-homogeneous materials like V_2O_3 and fully disordered materials like Si:P. (See G. A. Thomas, in "High Temperature Superconductivity", D. P. Tunstall and W. Barford, eds. (Adam Hilger, Bristol, 1991), p. 169.

11 May: Ordered, but unusual, metallic states: the e-h liquid, etc.

A comparison will be given of quasi-ordered systems, like V_2O_3, classic disordered systems, like Si:P, the high T_c oxides, and some relatively order, but interesting systems, like the electron-hole liquid, and metallic Bi_2Te_3. Emphasis will be placed on unsolved problems. (See J. C. Hensel et al., in "Solid State Physics, Vol. 32," Seitz, Turnbull, and Ehrenreich, Eds. (Academic Press, New York 1977; see also G. A. Thomas et al., Phys. Rev. B 46, 1553 (1992).)

Observation of the gap and kinetic energy in a correlated insulator

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Fundamental energies are determined optically for an ensemble of correlated electrons in an antiferromagnetic insulator, V_2O_3. The observed variation of the energy gap and the kinetic energy are compared quantitatively to some approximate solutions of the Hubbard Hamiltonian.

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A crystal with a partially-filled band should be a metal at low temperatures. In the case where the band is expected to be half-filled, but the crystal is observed to be an insulator, Mott [1] and Hubbard [2] have suggested that the band could have been split by the Coulomb repulsion among the electrons. Alternatively, Slater [3] suggested that antiferromagnetic interactions alone could open an energy gap to produce the insulator. Recently, new, approximate solutions [4] [5] [6] [7] of the Hubbard model containing both these ideas have been studied extensively. The motivation of our experimental study is to compare these ideas with the optical spectra of a correlated system.

Important questions have been raised about the applicability of a simple model to the real system, V_2O_3. One question is the role of charge-transfer excitations. Our measurements of the optical conductivity for V_2O_3 over a wide energy range (from 0 to 12.5eV) are shown in the inset to Figure 1. (It is an insulator at low temperatures, in agreement with previous results [1] [8] [9]). Band-structure calculations [10] (neglecting Coulomb interactions) show that the metallic phase of V_2O_3 has a range of V-V transitions (from predominantly V initial states to predominantly V final states) up to about 3.5eV (arrow), and a range of V-O transitions at higher E. We conclude that the Mott-Hubbard type of excitations (rather than the charge-transfer excitations) predominate at low E, so it is reasonable to neglect the charge-transfer excitations. However, Mott [1] and others [6] have argued that a simple version of the Hubbard model will be inadequate because of the clearly established roles of magnetism and lattice effects. Nonetheless, others [8] including Anderson [12] for example, aware of the magnetism and structure, have suggested that the model does apply to V_2O_3 with an effective Coulomb interaction energy. Regarding the importance of magnetism, Brinkman and Rice [11], for example, have argued that the metallic state can be treated as it approches the insulating state by an approximation in which magnetic correlations are neglected. Similarly, Kotliar *et al.* [5] have argued that these correlations make a small, but important contribution near the metal-insulator transition in V_2O_3. We have chosen to study V_2O_3 to test the applicability of these various models.

Another motivation for our choice of V_2O_3 was that carefully characterized crystals [9] [13] [14] were available. We have measured the electronic kinetic energy in the insulating state and the optical energy gap, which, to our knowledge, have not been measured previously. We have also observed the variation of both the kinetic energy and the gap with the strength of the Coulomb interactions. Previously, an energy gap has been inferred from various measurements, such as the temperature dependence of the resistivity [8] [13] [14]. However, the only previous far-infrared optical measurements [15] showed a reduction in the low conductivity at low E but no energy gap. A similar reduction in the density of states has been observed in photo-emission spectra [16], also with no spectral region with negligible signal intensity.

We have made measurements with energy resolution less than one meV on crystals which we found to be very difficult to anneal, polish, and etch, with the additional difficulty that they crack on passing through the metal-insulator transition that occurs on cooling from room temperature. Based on optical and dc transport characterization of over 10 crystals, we have developed annealing and surface preparation procedures which yield reproducible spectra [17]. We have extended our reflectivity measurements from the far-infrared up to E=3.5eV (a frequency, ω, of about $27000cm^{-1}$) and used the measurements of Shin *et al.* [18] from 3.5 to 25eV in our Kramers-Kronig transformations to obtain the optical conductivity,

σ.

The main part of Figure 1 shows σ at low ω (and E) for two crystals of V_2O_3 in their low-temperature insulating phase. The measurement temperatures were less than half the metal-insulator transition temperature, T_c, for each sample. The open circles are for a nominally stoichiometric crystal with $T_c = (154 \pm 1)K$. The solid circles are for a sample that was annealed differently to introduce V-vacancies and a reduced $T_c = (50 \pm 1)K$. The effect of this annealing is qualitatively similar to an effective pressure [14], although there is undoubtedly some disorder in the system [1]. This change with annealing differs from doping a rigid band without disorder (often discussed in the theoretical literature [4] [5]) which can introduce conducting states into a filled band, and it also differs from disordered doping which introduces impurity states into the gap [1]. We see negligible absorption except that due to phonons in the energy gap, and our σ extrapolated to E=0 agrees with the (essentially zero) measured dc conductivity, σ_{dc}, of similarly prepared samples.

Qualitatively, the spectra show an energy gap, 2Δ, with a "soft" edge and a broad peak at higher energy. This type of spectrum resembles that predicted by various models [5] [7] [19] [20] with no intersite spin correlations. This behavior differs from our expectation for a Slater antiferromagnet [3], where we would expect a $E^{-1/2}$ divergence in the density of states at the band edge which would produce a σ rising sharply as $E^{1/2}$. Given the qualitative resemblance to the weakly-magnetic model, we shall proceed to compare the data of Figure 1 with the model quantitatively.

We expect that the peak in σ arises from a superposition of the states in the (filled) lower Hubbard band and the (empty) upper Hubbard band, with unperturbed band edges. If this single-particle density of states rises as $E^{1/2}$ near the band edges, we estimate that σ will rise as $E^{3/2}$ just above 2Δ. We then determine the values of 2Δ using a fit to this form (solid lines, Figure 1.):

$$\sigma = \sigma_0(E - 2\Delta)^{3/2}, \tag{1}$$

where σ_0 is a constant related to the average kinetic energy which we shall discuss below. The corresponding values of T_c, σ_0, and 2Δ are [154K, $9.71\text{x}10^{-4}(\Omega - cm)^{-1}$, (0.66±0.05)eV] and [50K, $2.27\text{x}10^{-3}(\Omega - cm)^{-1}$, (0.09±0.05)eV].

The standard definition of the theoretical Coulomb repulsion energy, U, is the energy difference between the peaks of the lower and upper Hubbard bands in the single-particle density of states. For relatively large U, the absolute E of the maximum in the optical σ, U_m, (see arrow in Figure 1) corresponds [7] [19] [20] to U. The accuracy in determining U_m is limited by the uncertainty in our reflectivity measurements and in our Kramers-Kronig transformations (as in the case of 2Δ). The approximation of mapping U_m on to U is not included in our error estimate. Our values of T_c and U_m are [154K, 1.27±0.05eV] and [50K, 0.98±0.05eV].

The hopping energy, t, which appears in the usual form of the Hubbard Hamiltonian is proportional to the band-width, D, through the number of nearest-neighbor hopping sites. We again assume symmetric bands and define the full-width of the single particle bands to be 2D, so the half-width at half-maximum of the peak in the measured σ, D_m, corresponds to D. (See the energy difference indicated by the arrow labelled D_m in Figure 1.) The uncertainty is similar to that in U_m, giving values of T_c and D_m of [154K, (0.31±0.05)eV] and [50K, (0.47±0.05)eV]. These narrow band-widths are comparable to band-structure

calculations for individual bands in the d to d manifold [10], and the increase in D_m in the lower T_c sample is consistent with the idea of an increasing effective pressure that increases the overlap of the atomic wave functions.

We plot the optical measurements of the energy gap (normalized to D_m) as a function of the experimental characteristic energy ratio, U_m/D_m, (solid points, bottom scale) in Figure 2. For additional measurements of the gap, we have used dc results from a series of samples with different stoichiometry [13] and applied pressure [14]. These measurements determined the excitation energy, Δ_{dc}, from the slope of the logarithm of the σ_{dc} as a function of the inverse temperature. We find that, for samples with $T_c = (154 \pm 4)K$, the typical value of $2\Delta_{dc}$ is about $2\Delta/1.7$, and we interpret this smaller transport value as indicating that the chemical potential is pinned at a weak impurity level (not apparent on the scale of Figure 1), rather than floating at mid gap. Therefore, we have scaled the values of $2\Delta_{dc}$ by 1.7. The values of U_m and D_m cannot be determined by dc measurements. Therefore, we have used the measured values of T_c to estimate these energies for the dc data by interpolating between the optical values. We assume $U_m/D_m = (U/D)_0(1 + [T_c/T_0]^3)$ and find T_0 =152K and $(U/D)_0 = 2.01$ by fitting to the optical data. We have chosen this T_c^3 functional form because we can fit the dc data to

$$2\Delta_{dc} = 2\Delta_0(T_c/T_0)^3, \tag{2}$$

with $2\Delta_0 = 0.4$eV. This T^3 variation may be due to the interplay between the ground state Coulomb energy and the lattice excitation energy at increasing T. We use a similar scaling to interpolate values of D_m for the dc data, $1/D_m = 1/D_0(1 + [T_c/T_D]^3)$, with $D_0 = 0.48$eV and $T_D = 188$K. Because of the scatter in the dc data, the functional form used to estimate the variation of U_m and D_m is not crucial to the rough comparison we wish to make here. This procedure yields the open points in Figure 2. The annealed series of samples [13] and the sample at a series of pressures [14] yield similar results. A linear extrapolation of all the data suggests a continuous gap closing at $(U_m/D_m)_c = 1.95 \pm 0.2$.

We compare these measurements with theoretical predictions for $2\Delta/D$ in Figure 2 by plotting the theoretical U/D on the upper scale, with the assumption (accurate for large U/D) that $U/D = U_m/D_m$. We consider four types of theoretical approaches: 1. perturbation [4] [21] about the exactly solvable limits, U/D=0 and U/D=∞, 2. Hartree-Fock mean-field [6], 3. slave boson mean-field [7], and 4. dynamical mean-field [5]. The first three can be applied directly to models in three spatial dimensions. The Hartree-Fock approach has been applied to a model incorporating many of the aspects of the crystal structure of V_2O_3. The fourth is strictly valid only in the limit of infinite dimensions, but may give a good approximation to three dimensions. It also has the advantage of validity for arbitrary U/D and inclusion of correlations not easy to incorporate in other approaches. Within each theoretical approach there are two simple limits for treating the magnetism. One limit assumes that the intersite spin correlations are zero, so the gap arises simply from U, which we shall refer to as the Hubbard limit. The second assumes simple, two-sublattice, antiferromagnetic order, so a large, additional contribution to the gap arises from the magnetism (the Slater limit).

Relatively large gaps are obtained in the Slater limit as shown by the dash-dot curve for the dynamical mean field theory [20]. The Hartree-Fock calculation [6] gives a lower result, 2Δ=0.3eV, as shown by the solid triangle plotted using U_m and D_m for the sample with

T_c=154K. (Because of the realistic structure used here, t e treatment of the magnetism is in between the two magnetic limits.) Smaller values of the ; ap also come from consideration of the Hubbard limit as illustrated by the dotted line from a slave Boson approximation on a simple cubic lattice [7], given approximately by $2\Delta/D_m = (U_m/D_m - 2.6)^{1/2}$. The solid line is from a calculation of the dynamical mean-field model in the Hubbard limit [20]. In this extreme limit, a metal-insulator transition occurs at U/D=U_{c2}/D = 3.05, with the formation of a band of extended quasiparticle states in the middle of a gap. However, this metallic state is only about 0.1% lower in energy than an insulating solution in which the gap closes continuously at U_{c1}/D = 2.15 as shown by the dashed line. It seems likely [5] [20] that a small magnetic contribution to the energy would stabilize the insulating solution without changing the values of 2Δ substantially. Such a small antiferromagnetic contribution could arise because the spin structure of V_2O_3 shows substantial frustration [22] with a mixture of ferromagnetic and antiferromagnetic, nearest-neighbor interactions.

The data of Figure 1 permit an additional test of the theory. Qualitatively, there is a dramatic increase in the spectral weight (area under the curve) with decreasing U_m/D_m. This weight provides a measure of the average electronic kinetic energy, $< \hat{T} >$. Kohn and subsequent workers [23] [24] [25] have shown that

$$< \hat{T} > / < \hat{T} >_0 = \omega_P^2/\omega_{P0}^2. \tag{3}$$

Here, we have normalized $< \hat{T} >$ and ω_P^2 to their values for the same band-width, but for U=0, $< \hat{T} >_0$ and ω_{P0}^2. Using the f-sum rule [23] [25], we determine ω_P^2 from the energy integral over σ. Since we find additional bands at higher E in V_2O_3, we have used a partial sum and integrated only over the lower E half of the conductivity peak. Assuming symmetric bands,

$$\omega_P^2 = 16 \int_0^{U_m} \sigma dE. \tag{4}$$

For the two data sets shown in Figure 1, we have the values of T_c and ω_P^2 of [154K, $(0.23\pm0.04)eV^2$] and [50K, $(1.2\pm0.04)eV^2$]. The uncertainty here contains the factors discussed above.

We evaluate ω_{P0}^2 following the calculations of Millis and Coppersmith [25], using a half-filled cubic lattice, a characteristic atomic kinetic energy, and the measured band-width and find

$$\omega_{P0}^2 = 1.4 D_m e^2/d_{VV}, \tag{5}$$

where d_{VV} is the average vanadium-vanadium distance in V_2O_3, 3.06 Å. For the two crystals, we have then T_c and $< \hat{T} > / < \hat{T} >_0$ of [154K, (0.11±0.05)eV] and [50K, (0.39 ±0.05)eV].

Using these determinations, we can compare the normalized average kinetic energy from experiment with that from the dynamical mean-field model in Figure 3 with no adjustable parameters. The calculated variation [20] of the kinetic energy for the (partly metastable) insulating branch of the Hubbard limit is shown as the solid and dashed curves, and the data are shown as solid points. The comparable calculation for the metallic state is similar to the result of Brinkman and Rice [11] and is shown by the dash-dash-dot line. The dynamical mean-field model (these two curves) is exact in the mathematical limit of infinite spatial

dimensions. The Hubbard model can also be evaluated for small U/D using perturbation theory in three dimensions [25] [4]. For this case, we find $< \hat{T} > / < \hat{T} >_0 = 1 - 0.16(U/D)^2$, which is shown as the dash-dot-dot curve. Similarly, for the large U/D limit in three dimensions [25] [21], we find $< \hat{T} > / < \hat{T} >_0 = 1.05U/D$ (the dot-dash curve) for the Slater limit and a result 1/2 as large (near the solid curve, but not shown) for the Hubbard limit (a nice example of the difference between these limits). All the curves show a suppression of the average kinetic energy (in addition to that expected from the band-width change) with increasing U/D, but the solid and dashed curves are in quantitative agreement with the measurements.

We conclude that, although we have measured a correlated antiferromagnet, we have not observed the large energy gaps and large kinetic energies expected in the Slater limit of approximate solutions to the Hubbard Hamiltonian. Instead, perhaps as a result of partial spin frustration, a partly metastable solution near the Hubbard limit is closest to our data. We consider this agreement to indicate that the dynamical mean-field model is quantitatively successful in describing the apparently continuous closing of the energy gap and the accompanying rise of the kinetic energy in insulating V_2O_3.

We wish to acknowledge helpful discussions with E. Abrahams, S. Coppersmith, L. F. Mattheiss, T. M. Rice, M. J. Rozenberg, D. J. Scalapino, D. Vollhardt, and particularly G. Kotliar. The work at The University of Chicago was supported by NSF DMR9204820; at Purdue University by MISCON on DOE grant DE-FG02-90ER45427.

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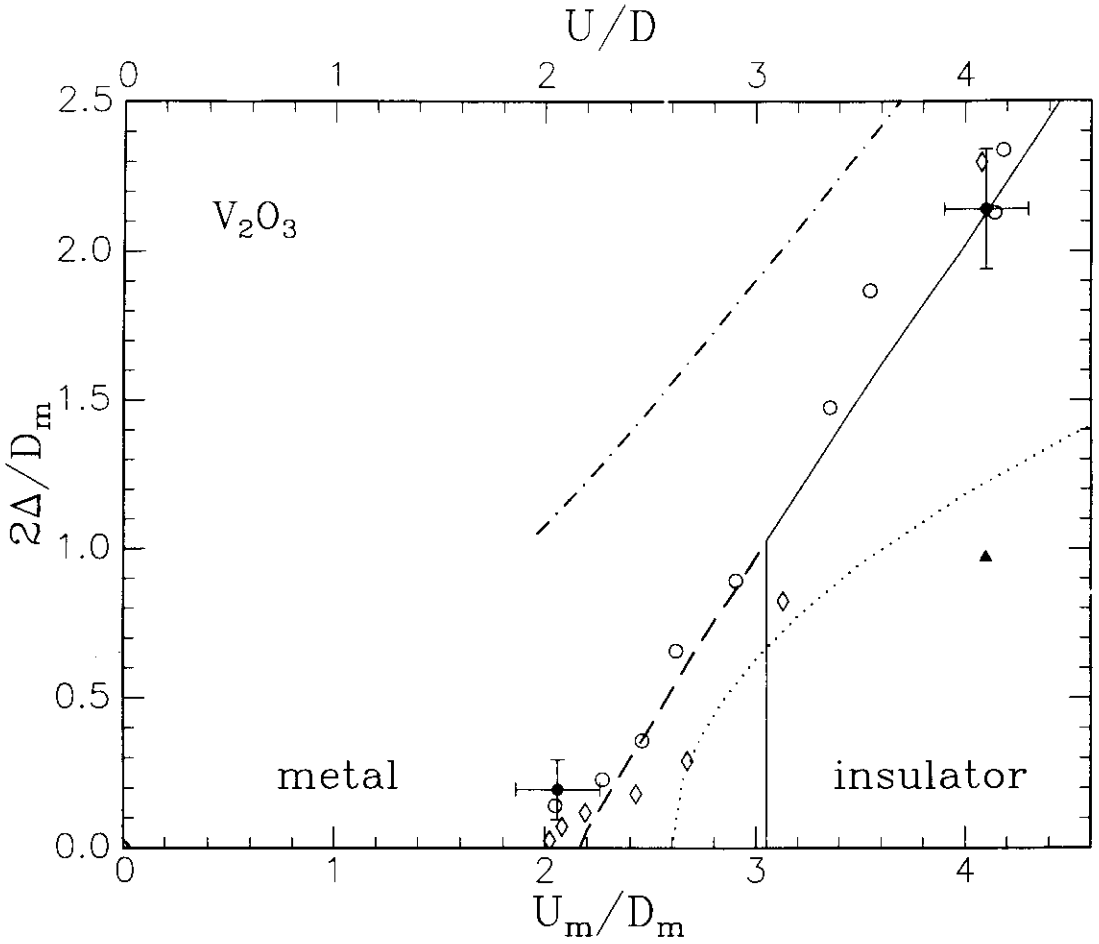
Figure captions:

Figure 1. Optical conductivity, σ, as a function of photon frequency, ω, (lower scale) and energy, E, (upper scale), for two crystals of V_2O_3 with metal-insulator transition temperatures, $T_c = 50$K (solid points) and 154K (open circles). For the upper curve, the energy gap, 2Δ, half-width, D_m, and peak energy, U_m, are indicated. The solid lines are fits to Equation 1. The inset shows a wider region of the sptectum for the sample with $T_c = 154$K with σ over a scale 0 to 5000 and E from 0 to 12.5eV.

Figure 2. Energy gap, 2Δ, normalized to the experimental band-width, D_m, as a function of the normalized experimental band energy, U_m, (bottom scale), for the optical measurements (solid circles), and dc measurements as a function of annealing (open circles) and as a function of pressure (open diamonds). The theoretical calculations of the normalized gap using the dynamical mean-field model [20] are plotted against the normalized theoretical Coulomb repulsive energy, U/D, (top scale) for the Slater limit (dash-dot line) and the stable (solid line) and metastable (dashed) branches of the Hubbard limit. A value calculated for V_2O_3 using the Hartree-Fock approximation [6] is shown as the solid triangle. A slave Boson calculation [7] in the Hubbard limit is also shown (dotted line).

Figure 3. Average kinetic energy, $< \hat{T} >$, normalized to the kinetic energy for U=0, $< \hat{T} >_0$, as a function of the same variables as Figure 2. The solid points are the optical measurements, (evaluated using Equation 4 and normalized using Equation 5). The dynamical mean-field theory [20] is plotted in the Hubbard limit for its stable branch (solid line) and metastable branch (dashed), and in the metallic state (dash-dash-dot). Perturbative calculations are plotted for large U/D in the Slater limit (dashed-dot) and for small U/D (dashed-dot-dot).


U/D
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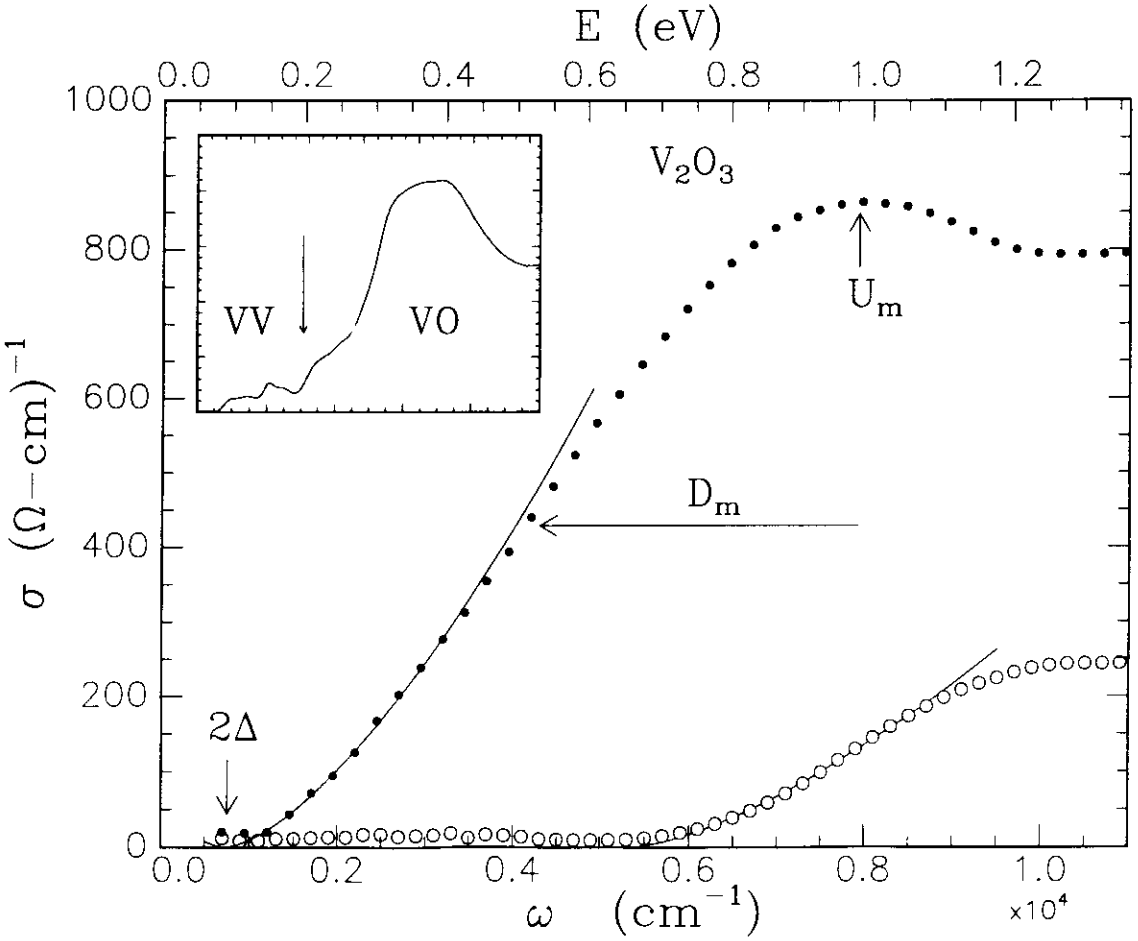
E (eV)
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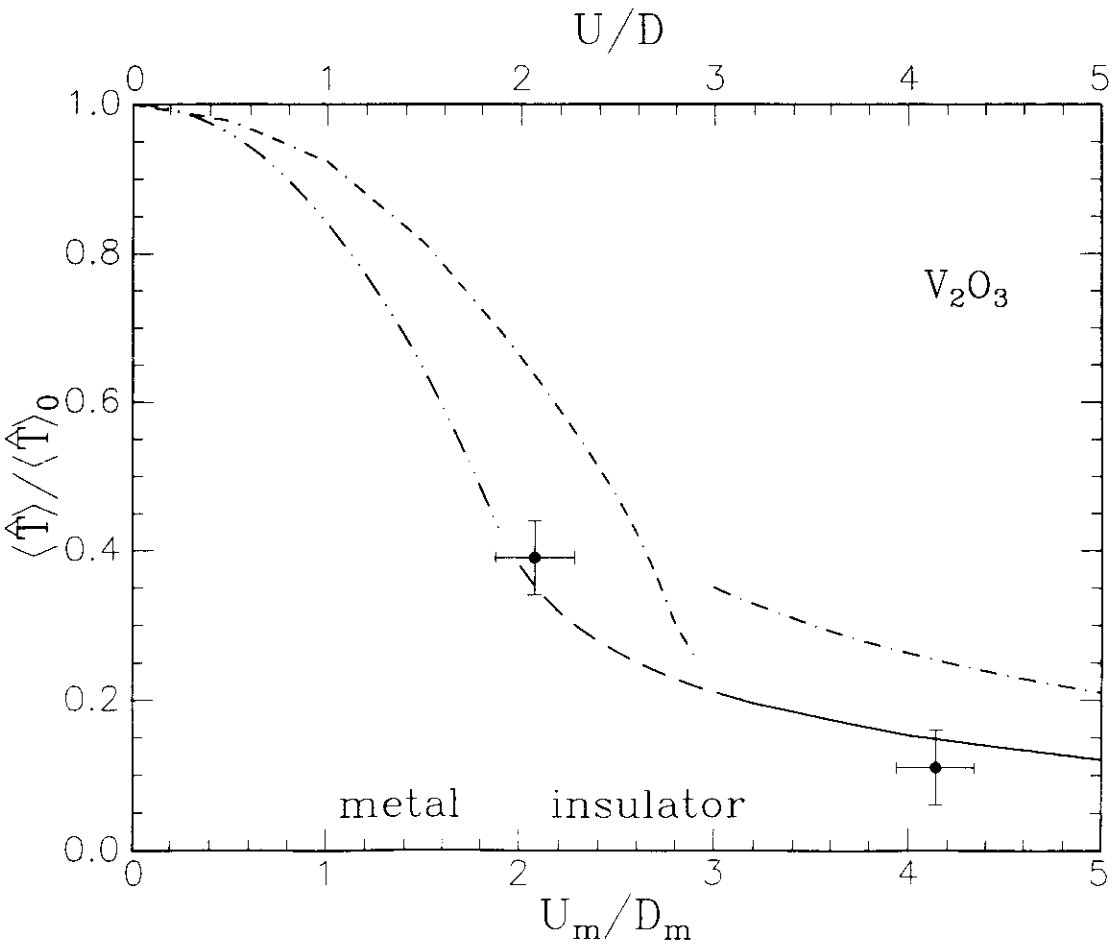
U/D
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$\langle\hat{T}\rangle/\langle\hat{T}\rangle_0$
V_2O_3
metal
insulator
U_m/D_m