AD-A224 830

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FIFTH QUARTER

RESEARCH PLAN

This quarter has been devoted to the study of the physical significance of the parameter Γ which can be obtained by Electrolyte Electroreflectance (EER) or by spectroscopic ellipsometry.

RESULTS

The generalized theory of electroreflectance (which has been carried out under separate funding) has permitted us to reconcile the Γ obtained by electroreflectance to the Γ obtained by ellipsometry.

However, it does remain that the value of Γ obtained either way can be as high as 120 meV as compared to the expected 70 meV. We have determined that this is due to the breakdown of the virtual crustal assumption and is in fact a quantitative measure of it. It turns out that the measured $\Gamma_m = \Gamma_o + kT + \Delta\Gamma$ where Γ_m is the measured linewidth, Γ_o is the expected 70 meV and $\Delta\Gamma$ measures the departure from the virtual crystal approximation. (See Attached Expose)

SIMPLE APPROXIMATION FOR EFFECT OF ALLOYING ON THE PHENOMENOLOGICAL LINEWIDTH Γ

Consider that $E_{cv}(\vec{k})$ is not a unique, sharply defined energy, but that for the absorption of a photon "locally", it depends on the local concentration c_{loc} averaged over a cluster of N atoms on the Hg-Cd sublattice.

$$E_{cv}^{loc}(\vec{k}) \approx E_{cv}^{loc}(\vec{k}_{cr}) + \frac{\hbar^2}{2\mu}(\vec{k} - \vec{k}_{cr})^2;$$

i.e., the dominant source of variation in $E_{cv}^{loc}(\vec{k})$ is the variation in the local critical point energy

$$E_o(c_{loc}) \equiv E_{cv}^{loc}(\vec{k}_{cr}).$$

Then, for $N >> 1$,

$$P(E_o) \approx (\sigma\sqrt{2\pi})^{-1} \exp\{-[E_o - E_o(c)]^2/2\sigma^2\}$$

with $\sigma^2 = E_1\, c(1-c)/N$,

where $E(c_{loc}) \approx E(c) + (c_{loc} - c)\, E_1$.

This leads to a replacement of the lineshape

$$L(E,\vec{k},\Gamma_o) = -[E - E_{cv}(\vec{k}) + i\Gamma_o]^{-1}$$

by $\mathcal{L}(E,\vec{k},\Gamma_o) = \int_{-\infty}^{\infty}\{E - E_{cv}(\vec{k}) - [E_o - E_o(c)] + i\Gamma_o\}^{-1} P(E_o)\, dE_o$

The only simple analytic result is obtained by replacing the Gaussian probability $P(E_o)$ by a Lorentzian probability. If one does this and chooses the Lorentzian probability to have width

$$\Gamma^1 = \sqrt{2}\sigma,$$

which follows from an expansion of e^{-u^2} as $[1 + u^2 + \ldots]^{-1}$, one finds that Γ_o is replaced by

$$\Gamma_m = \Gamma_o + \sqrt{2}\sigma = \Gamma_o + E_1\sqrt{2c(1-c)/N} + kT$$

This gives the following table:

$\Gamma-(\Gamma_o+kT)$	.04eV	.06eV	.08eV	.10eV
N	200	88	50	32

A better numerical approximation leads to values of N approx 40% larger.