Influence of temperature, strain, alloy composition, doping, and film thickness on the dielectric function of semiconductors

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Due to the pioneering work of Aspnes and Studna [1] and others following their example, the dielectric functions and interband critical point parameters of group IV semiconductors (C, Si, Ge, Sn, SiC) and III/V and II/VI compound semiconductors are fairly well established, as long as we consider these materials in bulk form, free of dopants and impurities, and at room temperature. This talk will give examples of how deviations from these ideal conditions affect the dielectric function and the interband critical points.

(1) With increasing temperature, critical points shift to lower energies and become broader. Also, excitonic enhancements become weaker, leading to a decrease of critical point amplitudes [2].
(2) Biaxial tensile stress (for example in strained epitaxial layers) shifts and splits critical points. These effects can be calculated within continuum elasticity theory using deformation potentials. The weight of the E_1 and $E_1+\Delta_1$ critical point amplitudes may also shift [3].
(3) The critical point energies in relaxed semiconductor alloys (such as $Si_{1-x}Ge_x$ or $Al_{1-x}Ga_xAs$) usually vary continuously, following Vegard's Law with small quadratic bowing corrections. Alloy composition can cause singularities, if the character of the band structure changes, for example a transition from a Ge-like to a Si-like band structure. Alloy scattering as well as statistical or macroscopic fluctuations of composition cause a broadening of the critical points. The amplitudes decrease due to a weakening of the excitonic enhancement. This also affects the excitonic phase angle. In strained semiconductor alloy layers, the effects of stress also have to be taken into account.
(4) Doping has three effects: First, the presence of free carriers adds a small Drude contribution to the undoped dielectric function. Second, the critical points red-shift, broaden, and become weaker due to the screening of the excitonic enhancement by the free carriers and scattering by ionized impurities. Third, due to band filling, the line shape of the critical points may change. We have shown this recently for heavily n-type germanium at low temperatures [4]. This effect can also be seen in transient ellipsometry spectra after femtosecond laser excitation with an 800 nm pump pulse [5].
(5) Finally, we believe that the dielectric function of ZnO varies with film thickness and depends on the choice of substrate. For example, ZnO on quartz is a type-I system, where the excitons are confined leading to an increase of the direct gap absorption. On the other hand, if ZnO thin films are grown on Si, the holes will quickly scatter into the Si substrate, which will lead to a decrease of the near-gap absorption and the refractive index. I hope to have more convincing data by October.

References:

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