

New Manifestation of Small-size Effect on Raman Spectra in Nano-semiconductors

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It was found that ZnO nano-particles (NPs) display amorphous features in Raman scattering spectra but crystalline ones in X-ray diffraction spectra. This is contrasted to the conventional wisdom that the phase structure of a material is unique, regardless of the measurement methods. It indicates that for a material with a few nano-meters, Raman spectra can not always considered as a tool to study phase structure and transition.

We discovered also a novel phenomenon in ZnO NPs that Raman frequencies of all optical modes are independent of particle sizes (Fig 1), as like in that discovered in InSb NPs in Ref 1. This is in contrast to the observed phenomenon in Si nanowires [2] and carbon nano-tubes [3]: Raman frequencies are dependent of particle sizes.

Since the amorphous Raman spectrum is relative to the vibrational density of states (VDOS), we calculated the VDOS with different sizes for two typical NPs, Si and InSb, in terms of the cluster model and show the results in Figs 2 and 3. The results exhibit that the peak frequency variation of VDOS bands with particle sizes emerge into two catalogs: one is the frequency to be changed for polar modes and the other is not changed for non-polar modes. This gives a theoretical confirmation for distinct features in Raman frequency with sizes observed in polar- and non-polar modes.

It is well known that the polar and non-polar vibrational modes are dominated by long-range electrostatic Coulomb (Flöhlich) and short-range deformation potential, respectively. Considered the samples are nano-scale, we can understand easily that the above distinct Raman features originate from the difference in active range of corresponding electron-vibration interactions.

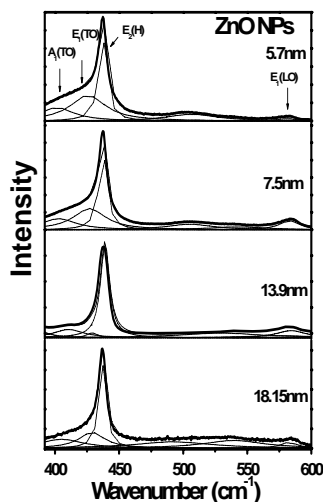


Fig 1 Raman spectra with sizes for ZnO NPs.

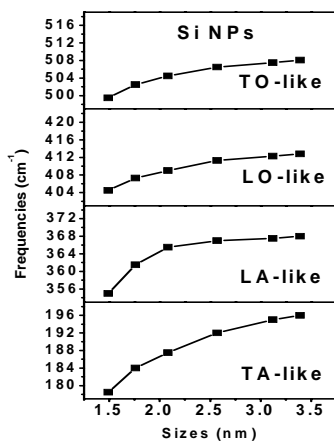


Fig 2 Calculated peak frequency of VDOS bands with sizes for Si NPs.

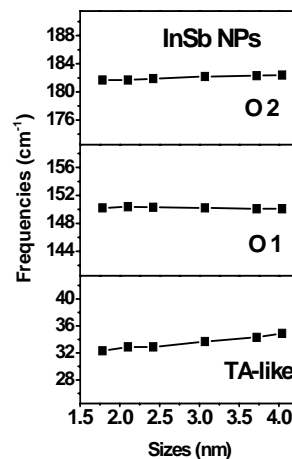


Fig 3 Calculated peak frequency of VDOS bands with sizes for InSb NPs.

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References

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