The Effect of Ge-Doping on Electronic and Lattice Vibrational Properties of FeGa$_3$

FeGa$_3$ is a doped intermetallic narrow-gap semiconductor often studied for its thermo-electric properties. It exhibits unusual magnetic, electronic properties and has a large thermopower coefficient. To study the electronic and lattice vibrational properties of FeGa$_3$ and FeGa$_{23}$Ge$_{0.16}$, we take optical measurements over a frequency range of 40 cm$^{-1}$ to 50000 cm$^{-1}$ for temperatures from 300K to 5K.

**Reflection**
- The undoped sample has low reflectance in the MIR range with sharp phonon modes in the low frequency region.
- Doping increases reflectance while forming a rough plasma edge. Addition of charge carriers screens the phonon modes at the lower frequencies.

**Conductivity**
- Fitting the optical conductivity with the Drude and Lorentz models shows an almost negligible Drude component in the undoped FeGa$_3$, but a clear emergence for Ge-doped sample.

![Conductivity Graphs](Conductivity Graphs)

- Using the LD fit underestimates DC-conductivity measured by direct four-leads electrical measurements.
- If we manually select the zero-frequency conductivity, we obtain very good agreement with DC-transport measurements.

**Optical Phonon Modes**

- Fe vibrations are not significantly affected by Ge-doping and can still be resolved clearly. Ga-vibrations shift to lower energy (Ge has heavier mass) and become highly disordered.
- In FeGa$_3$, the low frequency mode is very sharp and highly asymmetric (Fano line-shape). We need to extend the low frequency data for the doped sample.

**Magnetic Moments**
- We investigated potential changes in electronic band structure due to the magnetic ordering. There is a very small change in Mid-IR reflectance, with an almost undetectable effect on the absorption spectrum ($\alpha_\omega(\omega)$).

**Conclusion**
- Overall increase in reflectance, DC conductivity and Drude carriers due to doping.
- Selecting low frequency conductivity manually gives correct DC conductivities.
- Ga-vibrations shift to lower energy due to substitution of Ge at Ga sites, and they become disordered due to addition of carriers.
- Emergence of sharp phonon mode at low frequency with asymmetric Fano shape
- No significant effect on magnetic ordering.

**References**