RAMAPO COLLEGE OF NEW JERSEY

The Effect of Ge-Doping on Electronic and Lattice Vibrational Properties of $FeGa_3$

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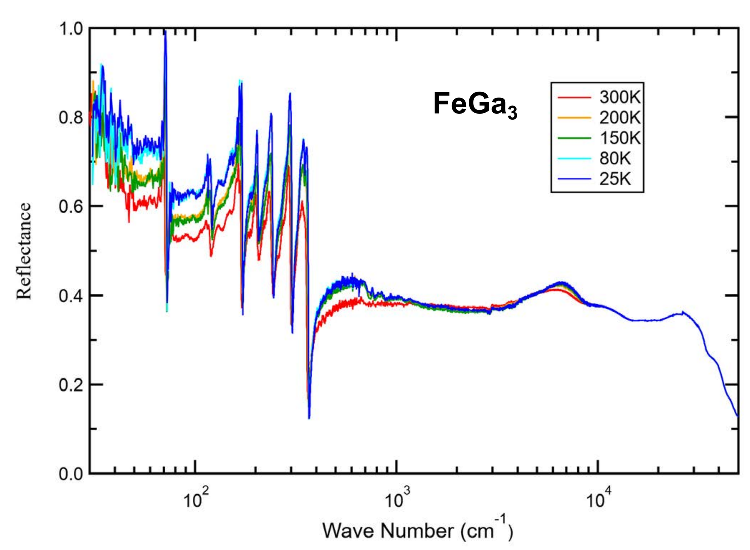
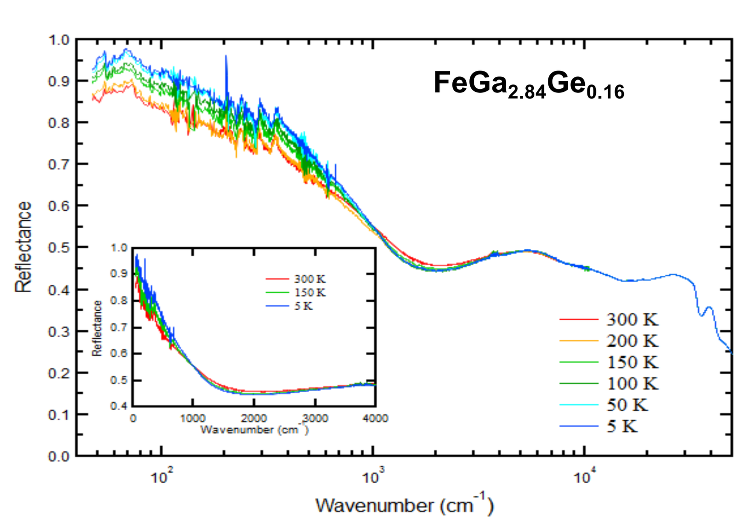
$FeGa_3$ is a doped intermetallic narrow-gap semiconductor often studied for its thermo-electric properties. It exhibits unusual magnetic, electronic properties and has a large thermopower coefficient. To study the electronic and lattice vibrational properties of $FeGa_3$ and $FeGa_{2.84}Ge_{0.16}$, 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.



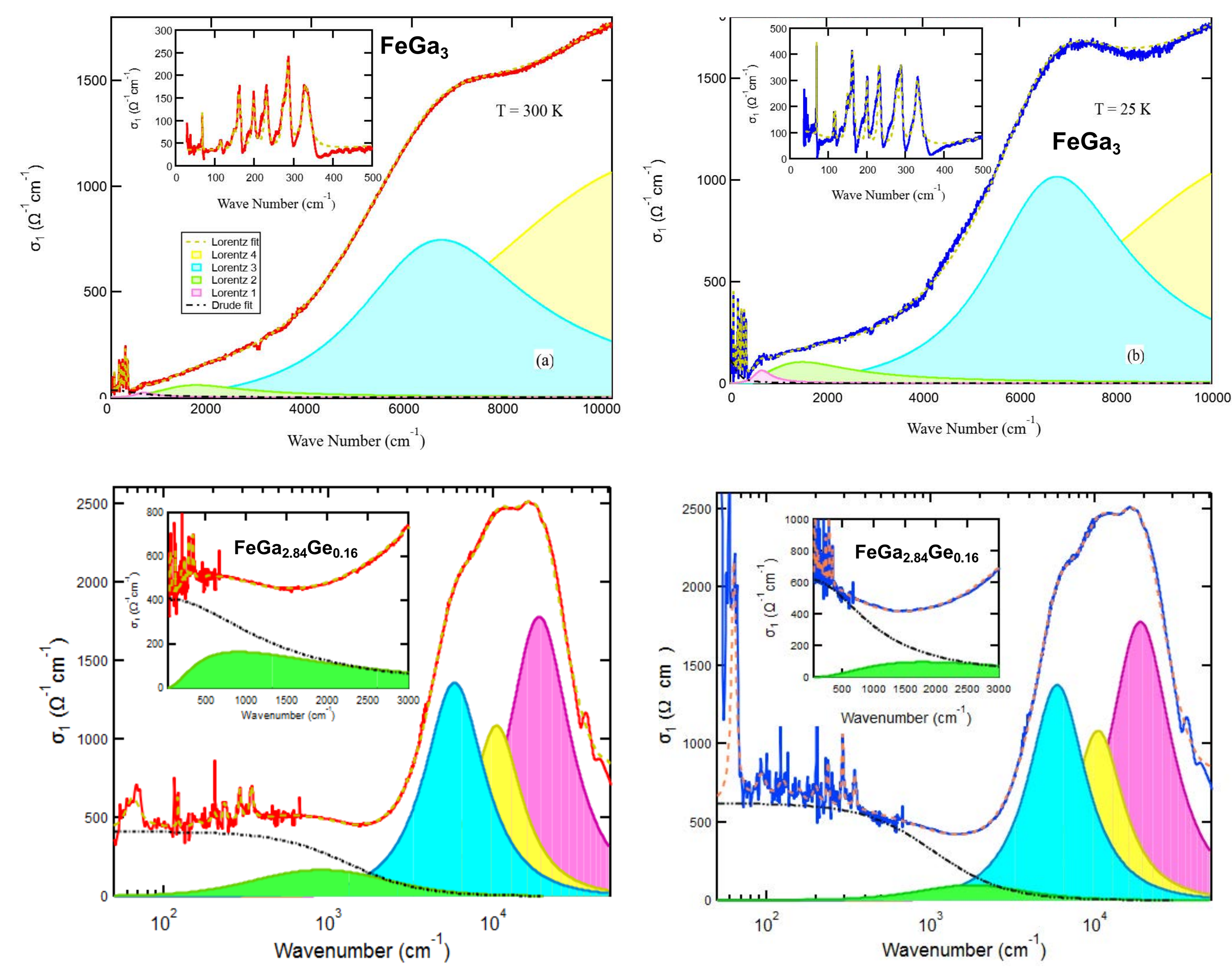


$$\tilde{\varepsilon}_r = \varepsilon_\infty - \frac{\omega_p}{\omega^2 + j\omega/\tau} + \sum_{i=1}^{N} \frac{\omega_{pe}^2}{\omega_{0i}^2 - \omega^2 - j\omega\gamma_i}$$

Lorentz-Drude fit

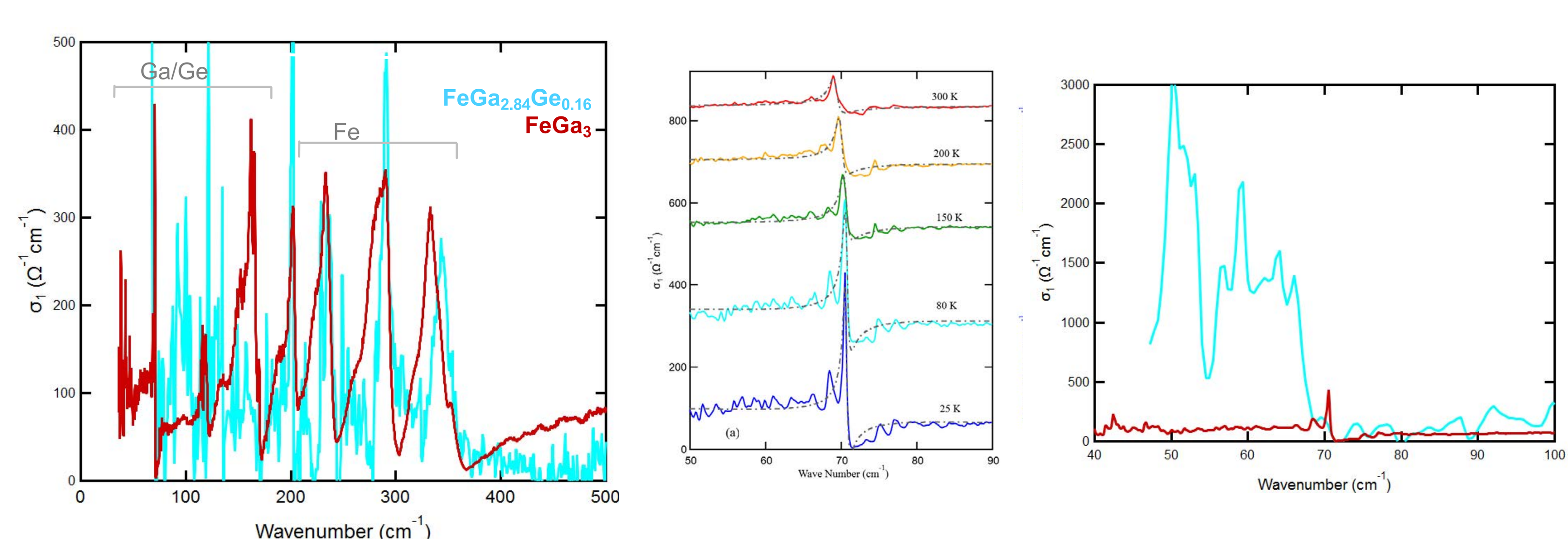
Conductivity

- 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.



- 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

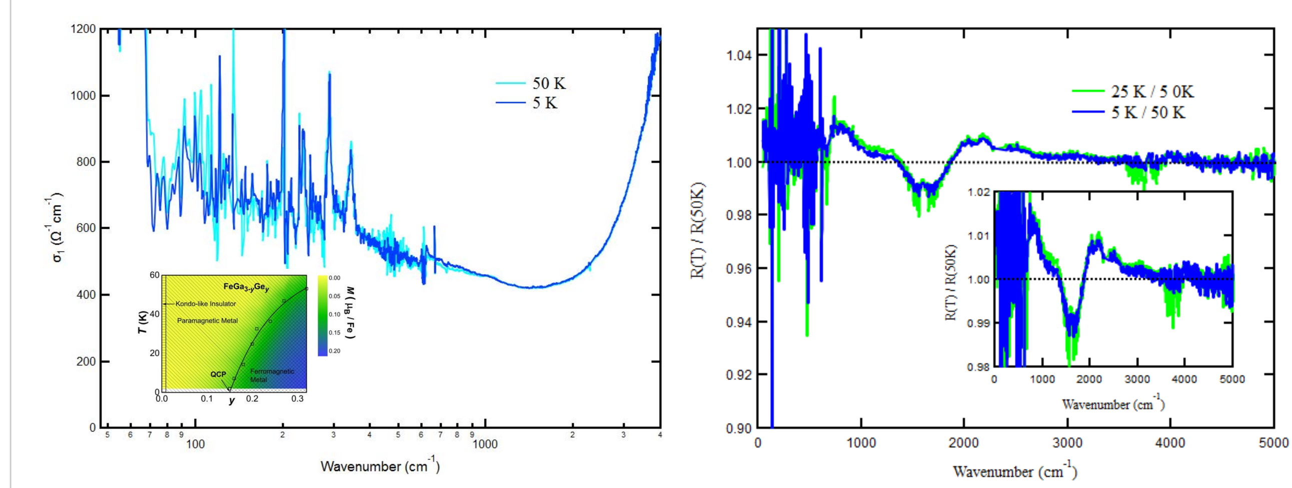
Optical Phonon Modes



- 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 ($\sigma_1(\omega)$).



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

- V. Ponnambalam and Donald T. Morelli. **Journal of Applied Physics** 118, 245101 (2015)
- Yao Zhang, et al. **PNAS** 115 (13) 3273-3278 (2018).