

# A New Unidentified Phonon State in SiGe Alloys Reproduced by Molecular Dynamics Simulation

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## Introduction

Predicting phonon behaviour is key for understanding thermal transport in semiconductor devices. The difficulties lie with observing and measuring phonon properties, owing to the challenges posed by instrumental limitations. Silicon-germanium (SiGe) is ideal for semiconductor fabrication, the alloy form is adopted to lower thermal conductivity but maintains electrical conductivity<sup>1</sup>. Yokogawa *et al.*<sup>2</sup> obtained the phonon spectrum of bulk SiGe alloys and observed a vibrational peak which has yet to be identified<sup>3</sup>. In this study, SiGe phonon dispersion relations were produced using molecular dynamics (MD) to investigate the origin behind this anomalous vibrational state.

## Simulation Methods

Bulk SiGe models were created with a cross-sectional diameter of 2.17 nm and a length of 16.3 nm. Periodic boundary conditions were imposed in the x,y,z crystallographic directions to emulate a 3D bulk system. Si<sub>55</sub>Ge<sub>45</sub> alloy consisted of Si and Ge atoms distributed randomly and Si<sub>50</sub>Ge<sub>50</sub> compound consisted of an Si-Ge-Si-Ge configuration. The mass difference was tested by maintaining the intrinsic masses of the Si and Ge atoms, but changing the potential parameters to give all the atoms the same potentials. The potential difference was also tested by giving all the atoms an identical mass but maintaining a difference for the potentials.

## Phonon Dispersion Relations

Using MD, the phonon dispersion relations were obtained by the Fourier transform of the spectral energy density (SED)<sup>4</sup>.

$$\Phi(\mathbf{k}, \omega) = \frac{1}{4\pi\tau_0 N_T} \sum_a \sum_b m_b \left| \int_0^{\tau_0} \sum_{n_{x,y,z}} \dot{u}_a(n_{x,y,z}; t) \times \exp[i\mathbf{k} \cdot \mathbf{r} \begin{pmatrix} n_{x,y,z} \\ 0 \end{pmatrix} - i\omega t] dt \right|^2 \quad (1)$$

where  $\Phi(\mathbf{k}, \omega)$  is the SED for the  $\mathbf{k}$  wavevector at  $\omega$  angular frequency,  $\tau_0$  the phonon lifetime,  $N_T$  the total simulation size,  $m_b$  the atomic mass of atom  $b$  displaced  $u$  in the  $a$  direction at a time  $t$ ,  $\mathbf{r}$  is the equilibrium positions of each unit cell,  $n_{x,y,z}$ .

## Results and Discussion

Si<sub>55</sub>Ge<sub>45</sub> (Fig.a) produced bands for the Si-Si, Si-Ge and Ge-Ge bonds, but an unaccounted-for vibrational mode also appears between the frequency range of 50 – 150 cm<sup>-1</sup>. This mode is in reasonable agreement with the additional peak observed by Yokogawa *et al.*<sup>2</sup>. The structure imposed with a mass difference produced a phonon dispersion relation almost identical to that of

the original Si<sub>55</sub>Ge<sub>45</sub> structure, as well as producing the unknown vibrational mode. A similar observation can be made for the structure simulated with a potential difference. Si<sub>50</sub>Ge<sub>50</sub> (Fig.b) did not produce the anomalous vibrational mode observed for the Si<sub>55</sub>Ge<sub>45</sub> alloys. Similarly, simulating this compound with a mass difference or a potential difference also yielded phonon dispersion relations without the anomalous peak.

## Conclusion

SiGe alloys and compounds were simulated in an attempt to investigate the origin of an anomalous peak displayed in the phonon dispersion relations. This anomalous peak was not observed when testing the Si<sub>50</sub>Ge<sub>50</sub> compounds but was observed when the Si<sub>55</sub>Ge<sub>45</sub> alloys were used. As Si<sub>50</sub>Ge<sub>50</sub> was simulated with an Si-Ge-Si-Ge configuration and did not produce the anomalous mode, it is speculated that a vibrational mode caused by the random configuration of atoms experienced in the Si<sub>55</sub>Ge<sub>45</sub> alloy is the origin of such a peak.

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## References

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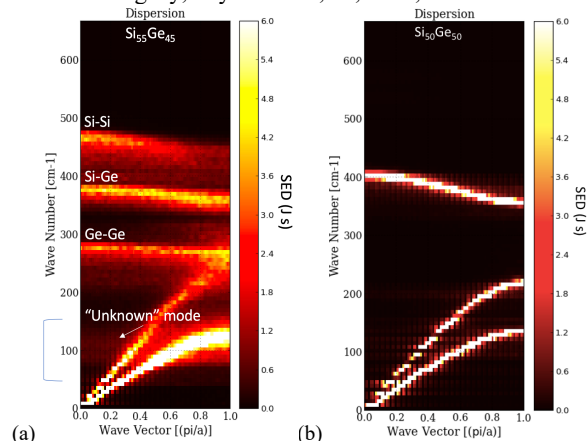


Fig. (a-b) Phonon dispersion relations for the Si<sub>55</sub>Ge<sub>45</sub> alloy (a) and the Si<sub>50</sub>Ge<sub>50</sub> compound (b).