



Alloy scattering of substitutional carbon in silicon: a first principles approach

M.P. Vaughan, F. Murphy-Armando and S. Fahy

Abstract

A method is developed to obtain the alloy scattering coefficients from first-principles band structure calculations. The method is then applied to find the electron scattering rates for substitutional carbon in silicon. Intravalley scattering is found to be the dominant process.

Motivation

The introduction of carbon into SiGe hetero-structure devices is of technological interest due to its dual roles of strain compensation and suppression of dopant diffusion. However, mobility measurements in Si(1-x)C(x) give conflicting results. Eberl *et al* [1] show an enhancement of the mobility believed to be due to the lifting of the degeneracy of the Δ valleys. Osten *et al* [2], on the other hand, show a degradation of the mobility that they attribute to carbon interstitials. Here we investigate electron scattering due to substitutional carbon on the mobility.

Alloy scattering

In the virtual crystal approximation (VCA) due to Nordheim [3], the potential of an alloy is taken to be an average of the constituent materials. The random deviations from this due to the substitution of different atomic species give rise to scattering. Our goal is to calculate the scattering matrix elements

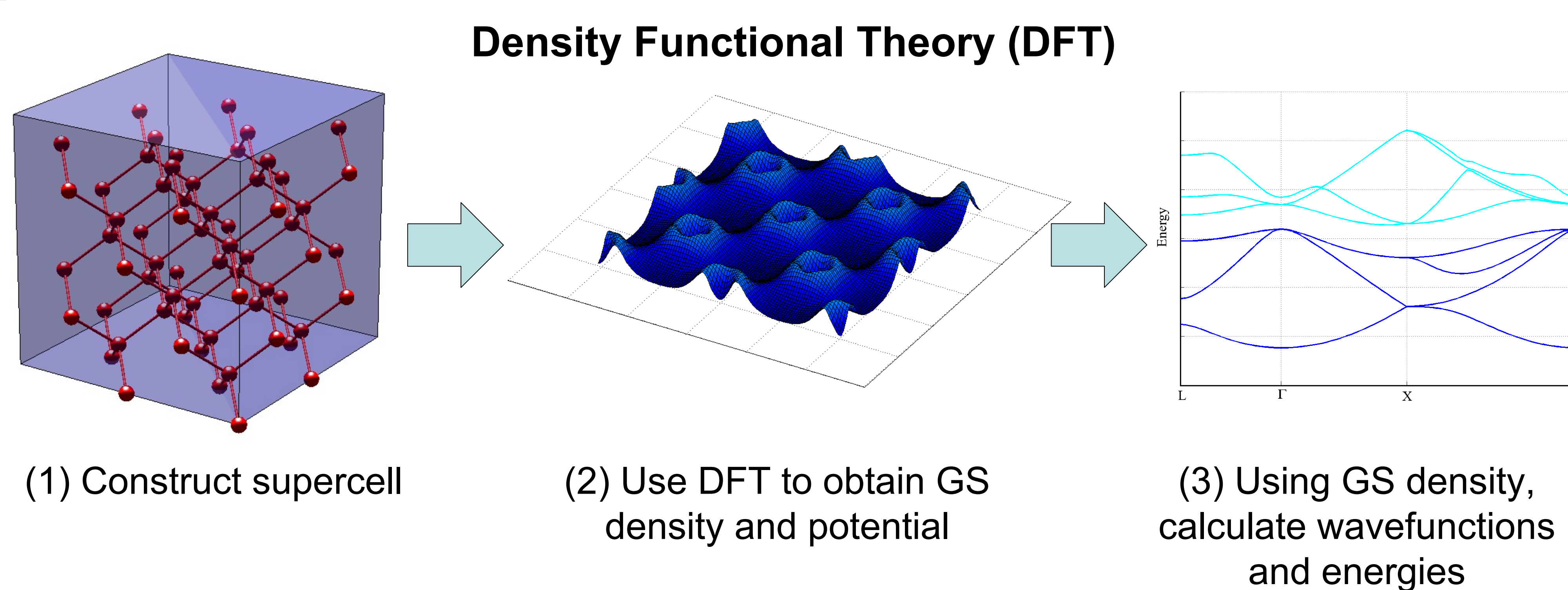
$$\langle \psi_{k'} | \Delta V | \psi_k \rangle$$

where ΔV is the difference in potential due to the substitution of one atomic species for another. We may then find the scattering rate

$$\frac{1}{\tau(E_k)} = \frac{2\pi}{\Omega} \left| \langle \psi_{k'} | \Delta V | \psi_k \rangle \right|^2 D(E_{k'})$$

where $\tau(E_k)$ is the carrier relaxation time and $D(E_{k'})$ is the density of final states. This expression may then be used in a solution of the Boltzmann equation to find the mobility.

Method



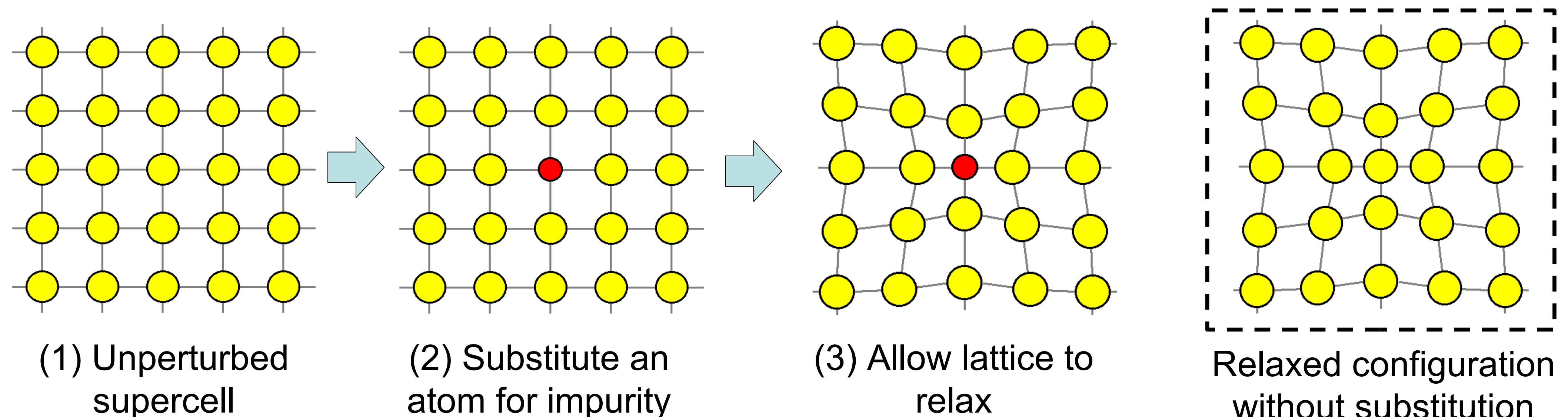
DFT

We use density functional theory (DFT) to calculate the ground state (GS) charge densities and potentials from first principles of large supercells for pure Si and with one Si atom substituted by a C atom.

These densities are then used to calculate the wavefunctions of the conduction band, from which we calculate the electron scattering matrices.

Chemical substitution and ionic relaxation

A schematic of the steps of chemical substitution and ionic relaxation is shown to the right. Firstly, we construct a supercell of pure Si. Next, we substitute a C atom for one of the Si atoms and calculate the ground state (GS) density. Finally, we allow the ionic positions to relax to their equilibrium configuration.



Results

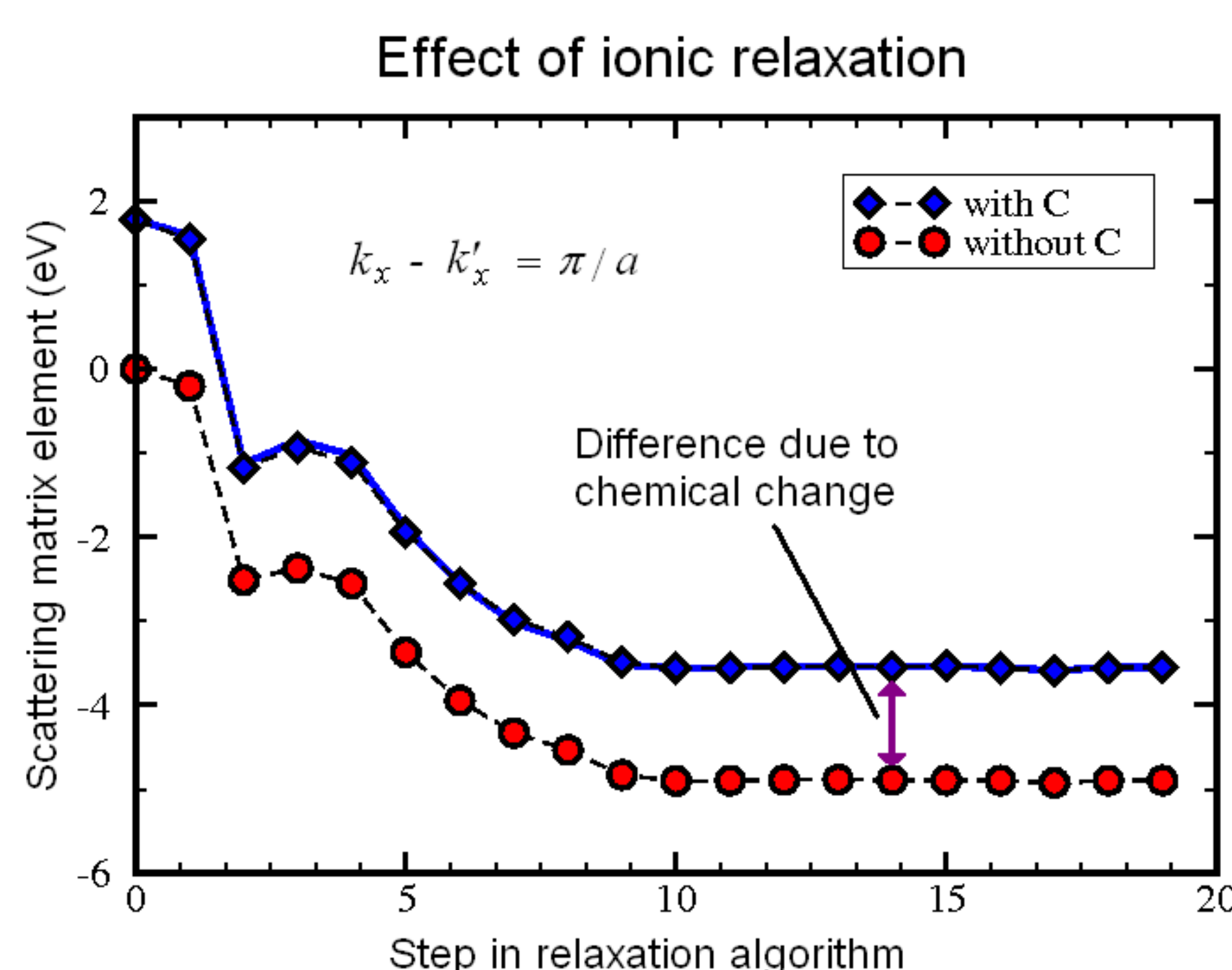


Fig. 1: Calculations at each step of the relaxation algorithm for the same ionic configuration with and without chemical substitution

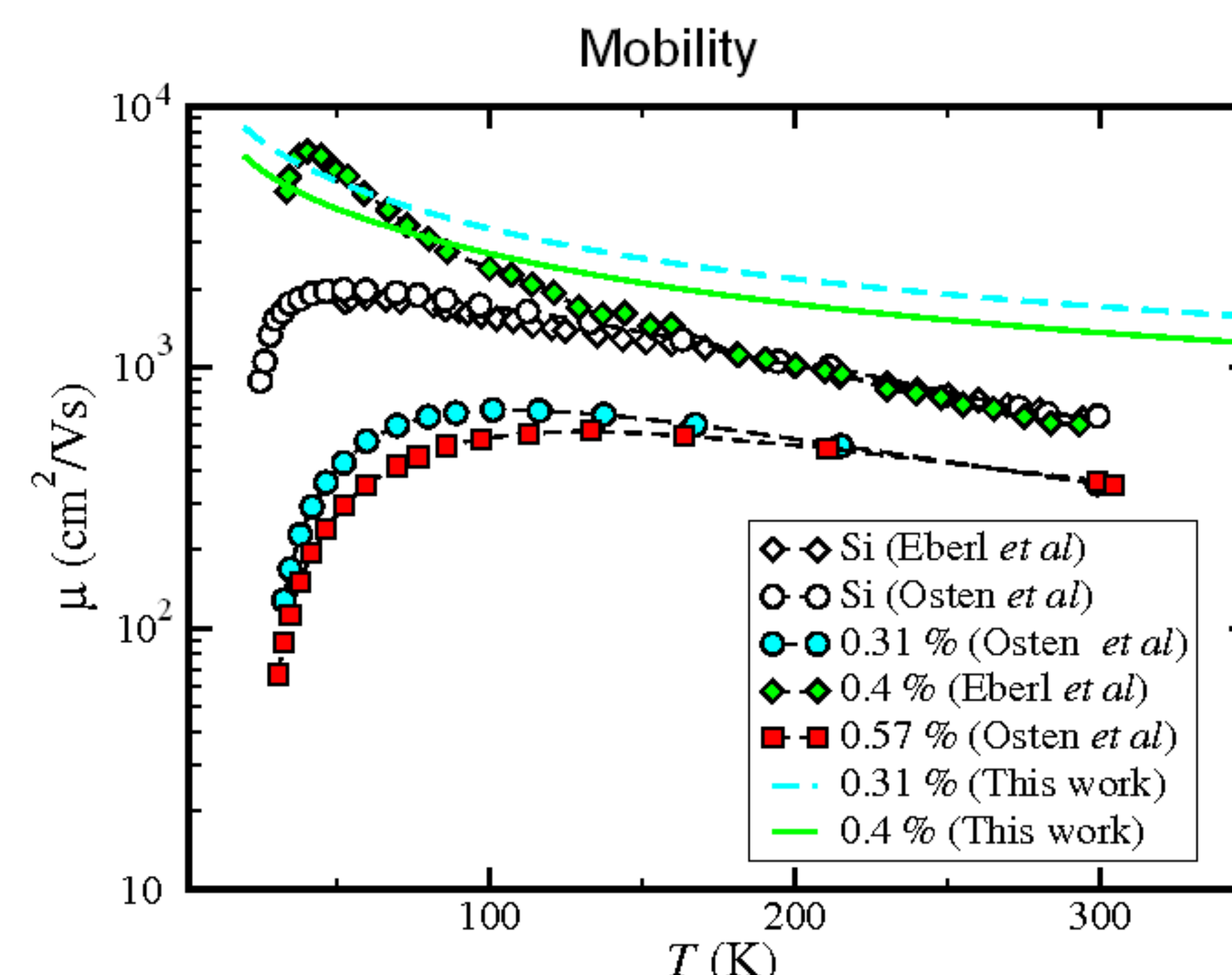


Fig. 2: Calculated (solid and dashed lines) and measured mobility. Calculated values are for the alloy scattering limited mobility only.

Conclusions

Our results yield 3 important conclusions:

1. Substitutional carbon in silicon does *not* produce an isolated state, unlike N in GaAs (not discussed in this poster)
2. The scattering matrices may be decomposed into two additive parts (see Fig. 1) due to:
 - a. chemical substitution
 - b. ionic relaxation
3. The scattering due to *substitutional* carbon is too small to account for the observed degradation in mobility seen in Ref. [2]. We therefore support these authors conclusions that this is due to C interstitials (see Fig. 2).

References

- [1] K. Eberl, K. Brunner and W. Winter, Thin Solid Films 294, 98 (1997)
- [2] H.J. Osten and P. Gaworzewski, J. Appl. Phys. 82, 4977 (1997)
- [3] L. Nordheim, Ann. Phys 9, 607 (1931)



Ireland's EU Structural Funds
Programmes 2007 - 2013
Co-funded by the Irish Government
and the European Union



www.tyndall.ie

