Electron Dynamics: Transport and Ultrafast Processes

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Research Group:

- Felipe Murphy-Armando (SiGe alloys)
- Eamonn Murray (ultra-fast optical excitation)
- Amanuel Teweldeberhan (vibrational probes of structure)
- Ivana Bosa (GaAsN - photoluminescence)
- Sian Joyce (SiGe alloys, NMR)
- John Buckeridge (GaAsN heterostructures - theory)
- Tassilo Dannecker (GaAsN heterostructures - expt.)

Tyndall Collaborators:

- Eoin O'Reilly
- Andy Lindsay
- Jim Greer

Recent Group Members:

- Henni Ouerdane
- Dermot McPeake
- Joe Stenuit (GaAsN alloys - structure, electr.)

Selected Highlights:

1. Intervalley alloy scattering in SiGe
2. Interatomic Forces in a Photoexcited Solid

Phys. Rev. Lett. **97**, 096606 (2006)
Science **315**, 633 (2007)

Alloy Scattering in SiGe

Felipe Murphy-Armando and Sian Joyce

Phys. Rev. Lett. **97**, 096606 (2006)
Phys. Rev. B **75**, 155201 (2007)

Ongoing Work - Charge Transport (SFI)

Area 1: General theory of scattering in disordered media
Area 2: ab initio calculation of alloy scattering in $Si_{(1-x)}Ge_x$
Area 3: Tight-binding calculation of scattering in $GaAs_{(1-x)}N_x$

General Goal: calculate bulk transport from first principles

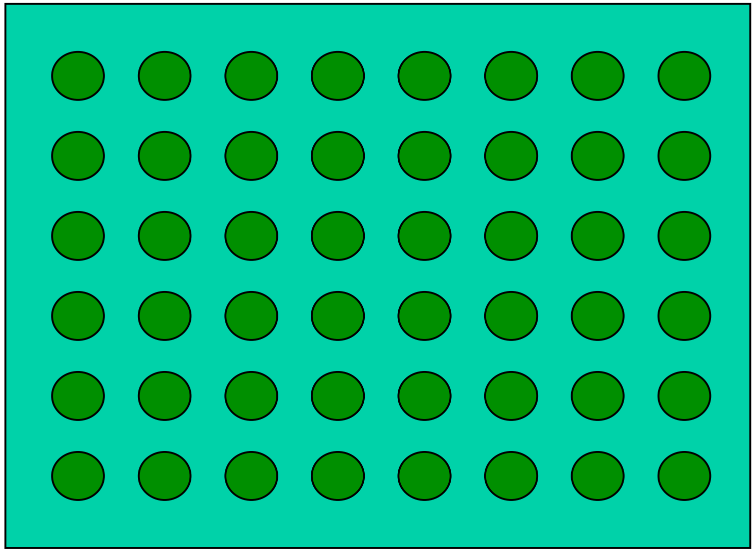
$Si_{(1-x)}Ge_x$:
* full alloy stability range ($0<x<1$)
* weak scattering
* "virtual crystal" good first approximation

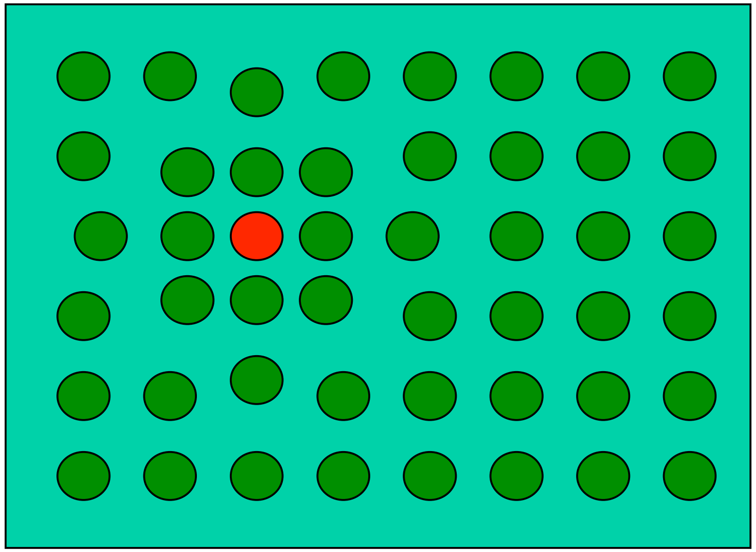
$GaAs_{(1-x)}N_x$:
* limited alloy range (dilute nitride, x~1-3%)
* very strong N scattering
* virtual crystal approximation not useful

Supercell Approach

Perfect lattice

Lattice with defect
(include lattice relaxation)





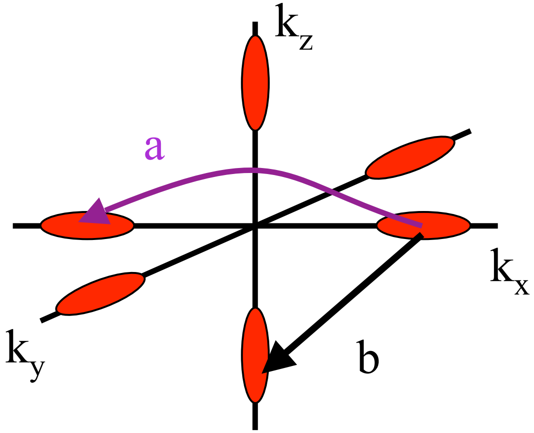
Calculate energy E_0 and □

Calculate E_1 and □

Scattering Matrix Element

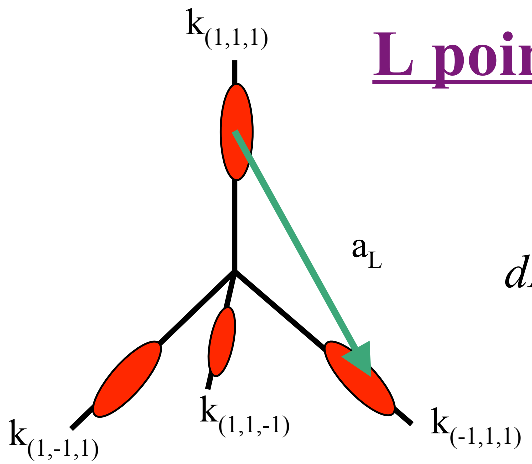
<□ | □H | □> = (E_1 - E_0) <□ | □>

Alloy Inter-valley scattering



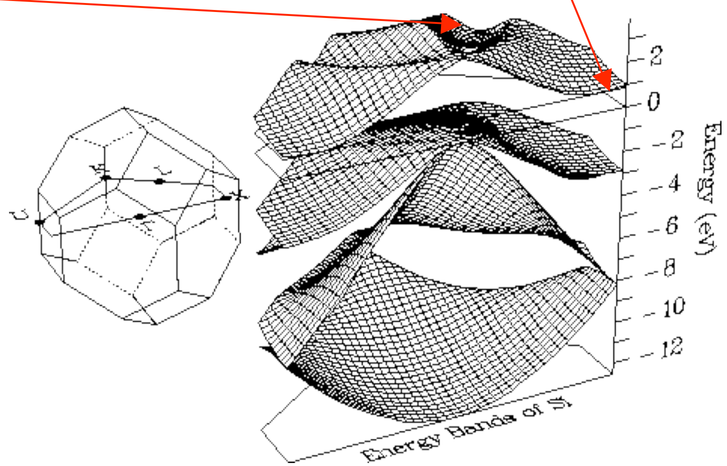
□ point

$$dH_{\square} = \begin{pmatrix} dE & da & db & db & db & db \\ da & dE & db & db & db & db \\ db & db & dE & da & db & db \\ db & db & da & dE & db & db \\ db & db & db & db & dE & da \\ db & db & db & db & da & dE \end{pmatrix}$$

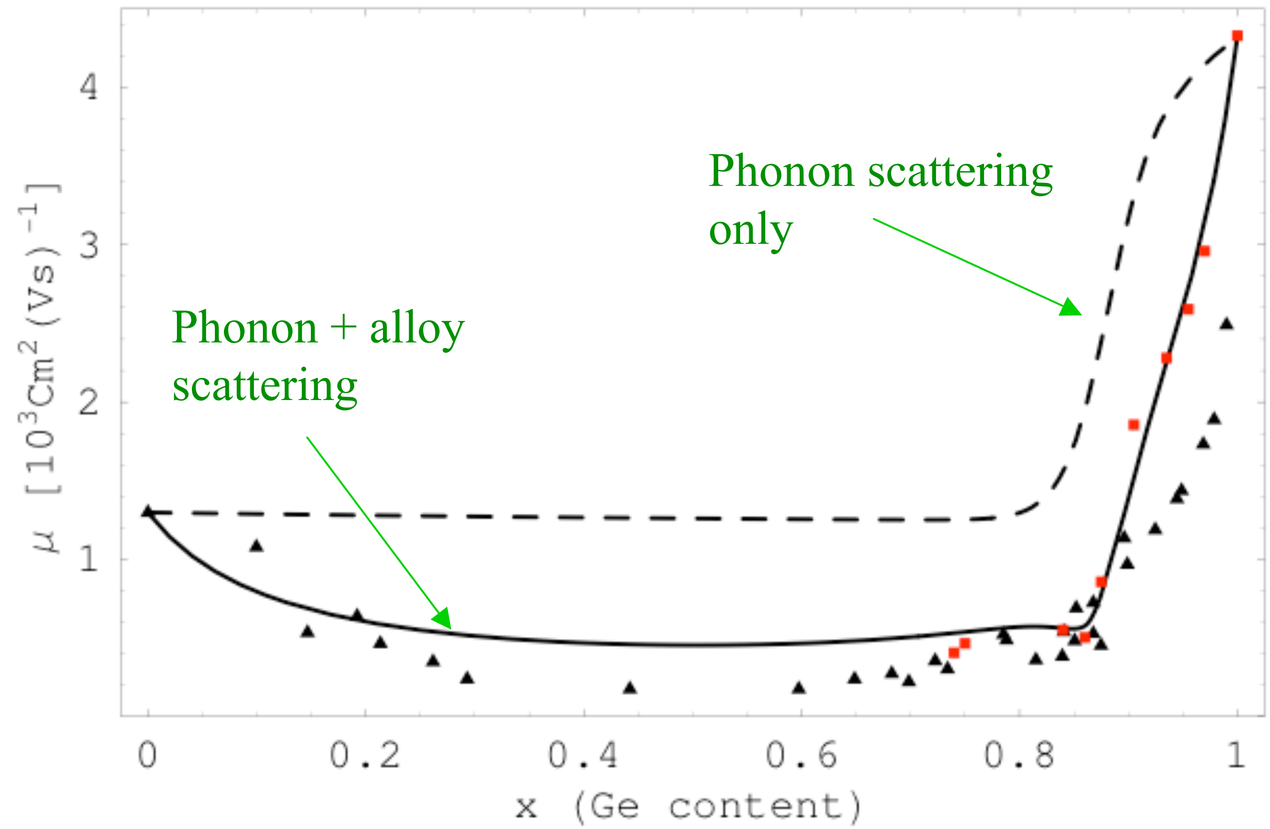


L point

$$dH_L = \begin{pmatrix} dE & da & da & da \\ da & dE & da & da \\ da & da & dE & da \\ da & da & da & dE \end{pmatrix}$$



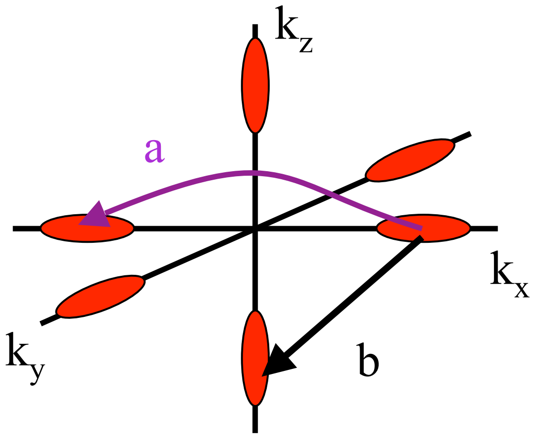
Results: Mobility from Alloy Scattering



Murphy-Armando PRL (2006)

Expts:
▲ G. Busch and O. Vogt, Helv. Phys. Acta 33, 437 (1960)
■ M. Glicksman, Phys. Rev. 111, 125 (1958)

Summary: SiGe Alloys



Inter-valley alloy scattering parameters well-determined for the first time

Future Applications:

1. Strained materials
2. III-V materials
3. Alloy scattering in SiGe nanoscale structures
4. Electron-phonon coupling in confined structures

Ultra-fast Carrier and Phonon Dynamics

Eamonn Murray

Goal: Understand energy relaxation processes in photo-excited materials

Phys. Rev. Lett. **93**, 109701 (2004)
Phys. Rev. B **72**, 060301(R) (2005)
Science **315**, 633 (2007)
Phys. Rev. B **75**, 184301 (2007)

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Tyndall National Institute

Collaborators

Theory:

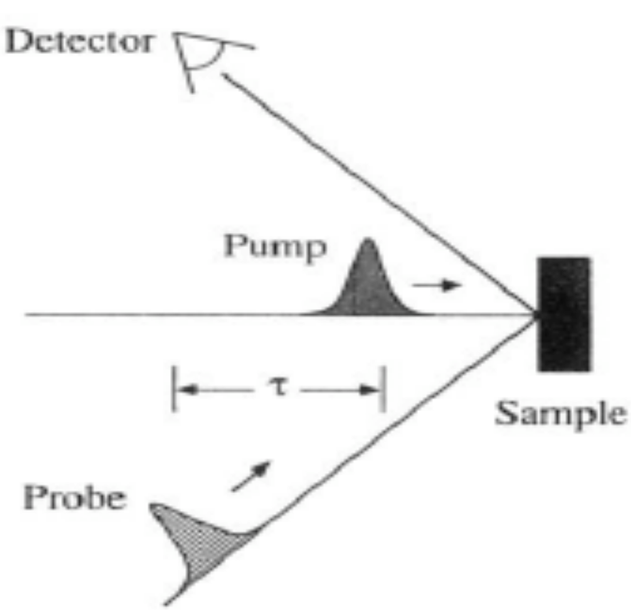
- Paul Tangney (Imperial College)
- Eamonn Murray
- David Prendergast (Berkeley, LBL)
- Tadashi Ogitsu (Livermore)

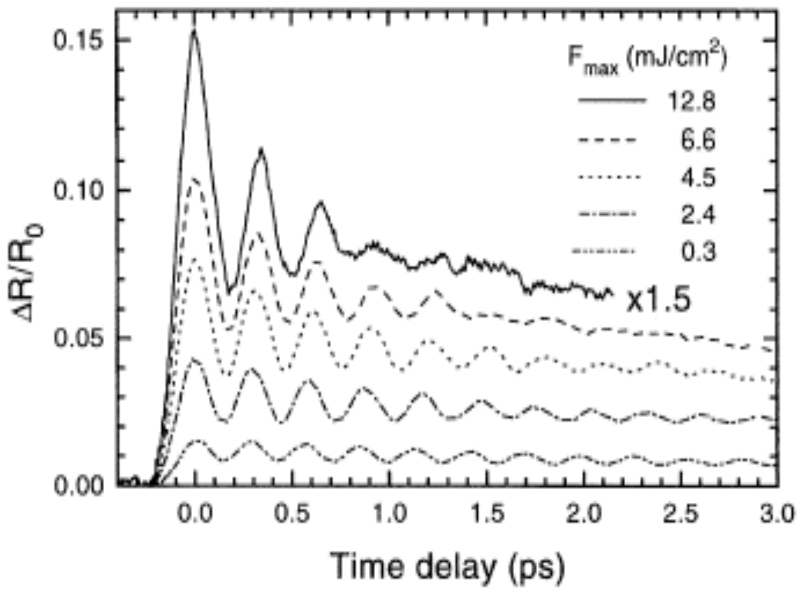
Experiments:

- David Reis (Michigan)
- David Fritz (Michigan)
- Jared Wahlstrand (Michigan)

- Phil Bucksbaum(Stanford)
- Roberto Merlin (Michigan)
- SPPS (Stanford, SLAC)
- FOCUS Center, Michigan

Pump-Probe Experiments





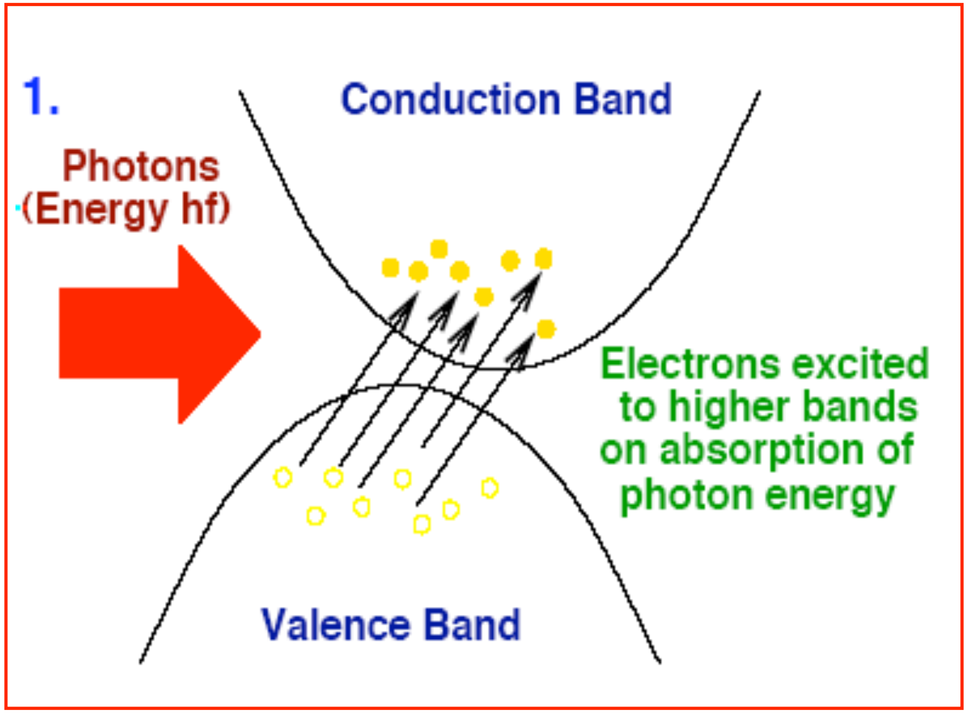
Expt. on Te - Hunsche et al. (1995)

- Changes in reflected probe pulse energy versus time delay between the pump and probe pulses
- Plasma and ionic motion alter reflectivity

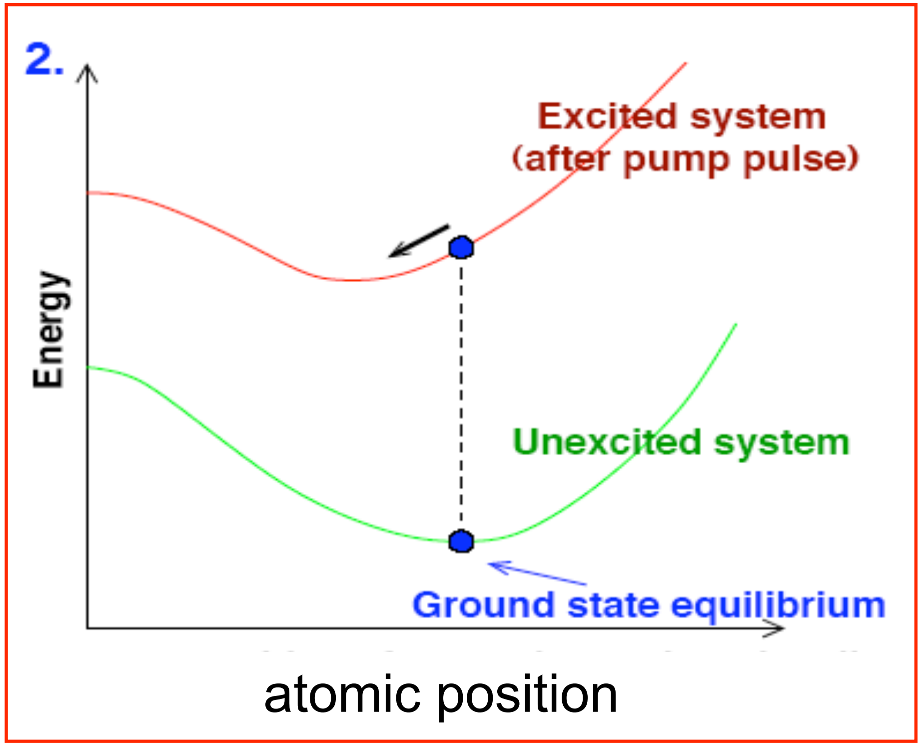
Displacive Photoexcitation Process

Creation of Electron-hole Plasma

Timescale: < 100 fs

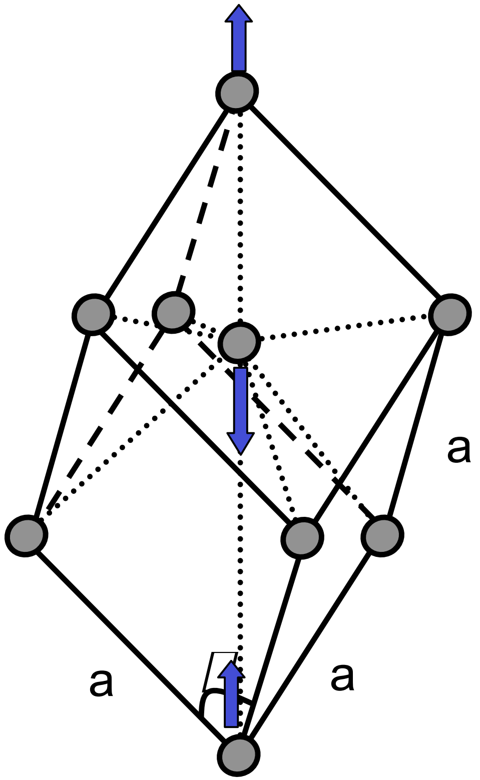


Altered Atomic Equilibrium

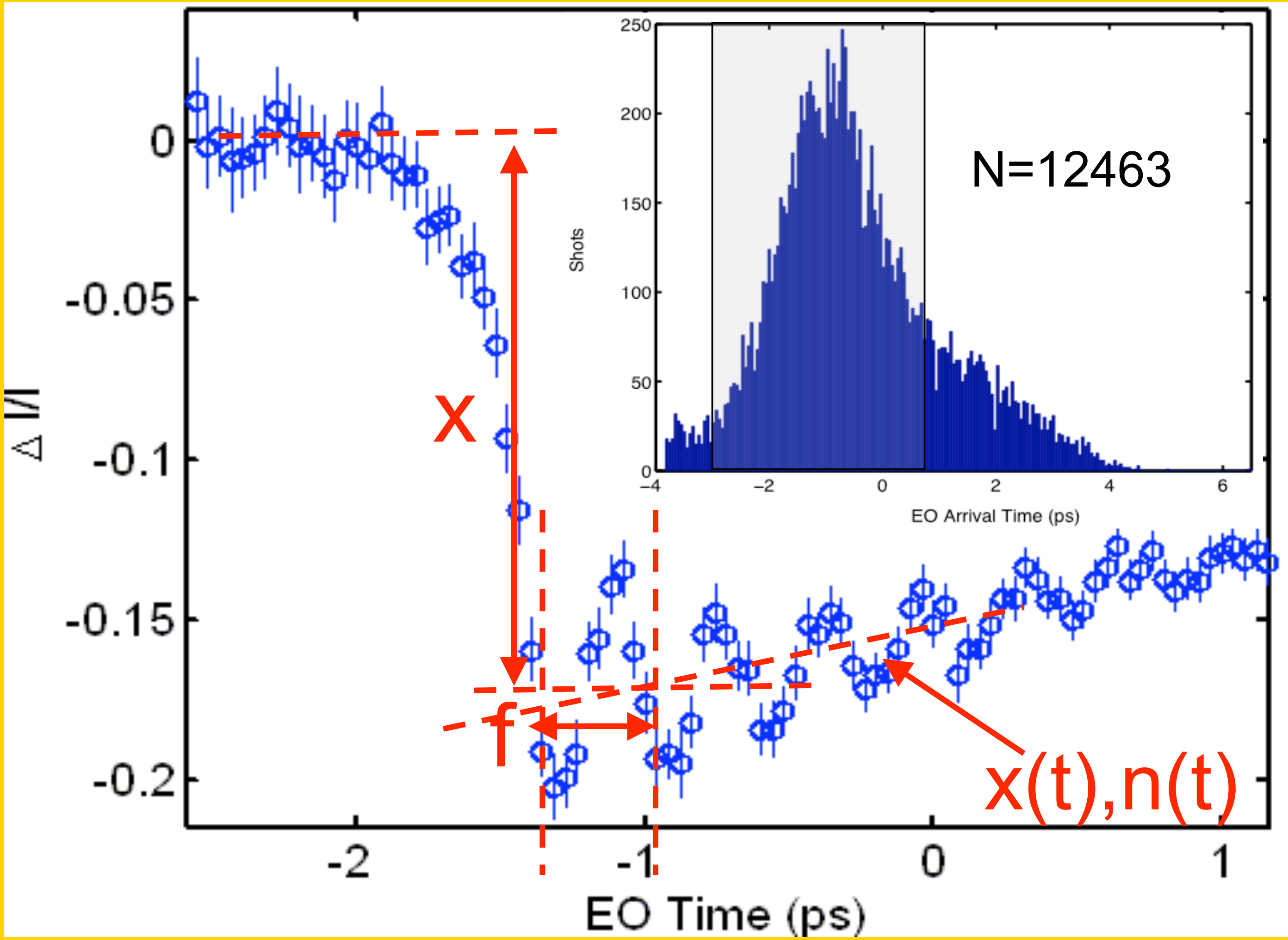


Note: does NOT include any coherent electronic polarization effects!

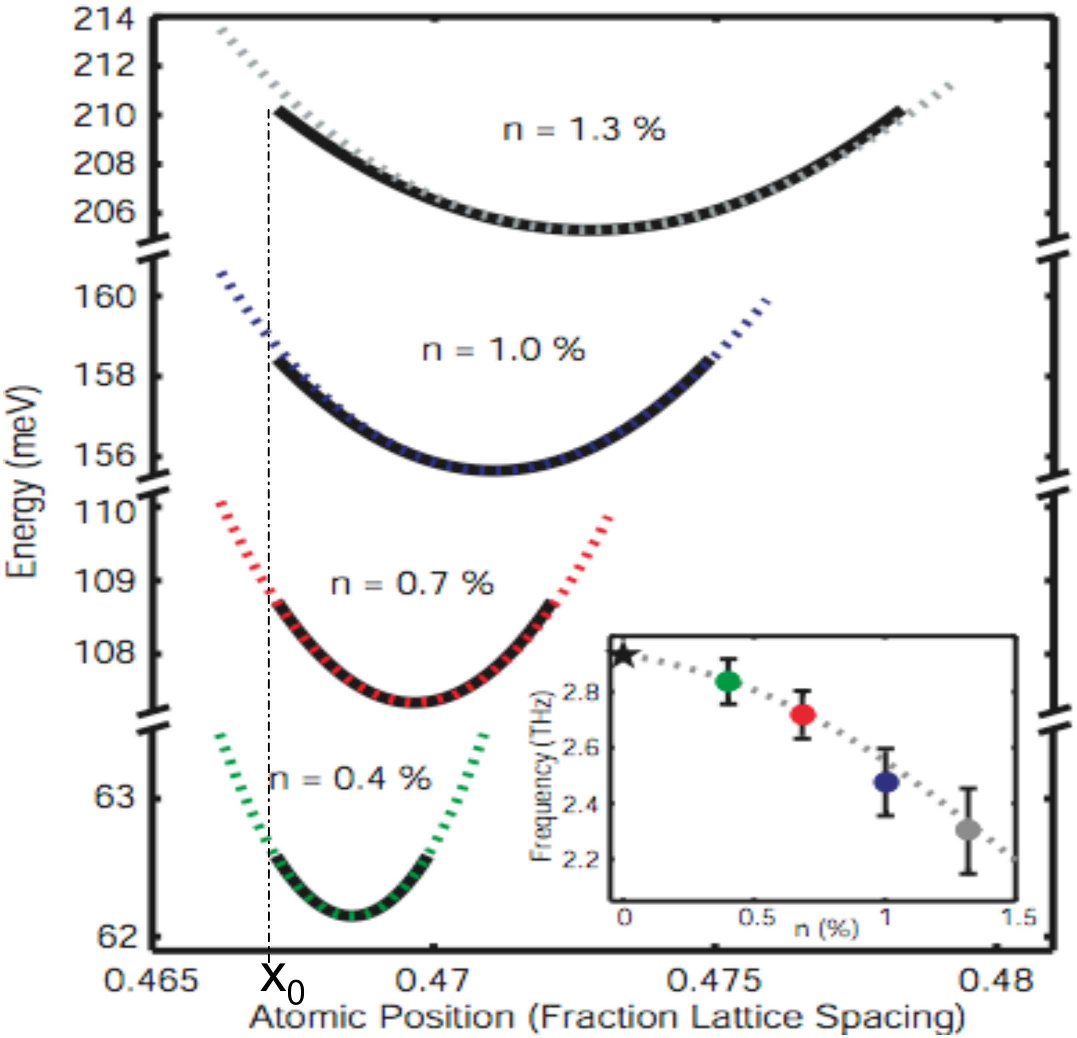
SPPS x-ray measurement of Bi dynamics



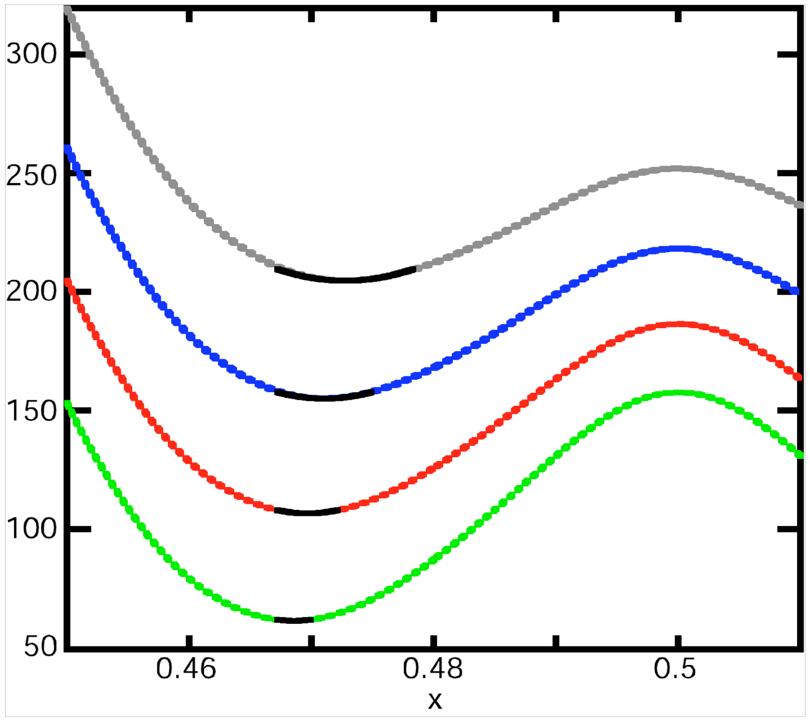
Fritz et al. (2007)



Measured Interatomic Potential of Bi

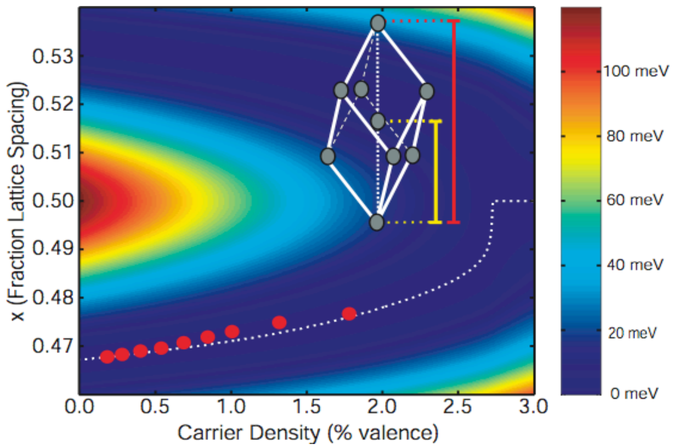


Calculated energy curves



Fritz et al. *Science (2007)*

Summary: Ultrafast Dynamics



First time Interatomic Forces have been Calculated and Measured for a photo-excited material

Future Applications:

1. Energy dissipation and phonon “bottlenecks” **4th year project!!**
2. Phonon probe of carrier inter-band relaxation
3. InSb phonon dynamics