Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Inverse band design of SiGe superlattices with direct band-gaps[1]

MAYEUL D'AVEZAC, NREL, JUN-WEI LUO, ALEX ZUNGER, NREL, Golden, Co, THOMAS CHANIER, University of Iowa — Integrating optoelectronic functionalities directly into the mature Silicon-Germanium technology base would prove invaluable for many applications. Unfortunately, both Si and Ge display indirect band-gaps unsuitable for optical applications. It was previously shown (Zachai *et al.* PRL **64** (1990)) that epitaxially grown $[(\mathrm{Si})_n(\mathrm{Ge})_m]_p$ (i. e. a single repeat unit) grown on Si can form direc-gap heterostructures with weak optical transitions as a result of zone folding and quantum confinement. The much richer space of *multiple-period* superlattices $[(\mathrm{Si})_{n_1}(\mathrm{Ge})_{n_2}(\mathrm{Si})_{n_3}(\mathrm{Ge})_{n_4}\ldots Ge_{n_N}]_p$ has not been considered. If $M = \sum n_i$ is the total number of monolayers, then there are, roughly, 2^M different possible superlattices. To explore this large space, we combine a (i) genetic algorithm for effective configurational search with (ii) empirical pseudopotential designed to accurately reproduce the inter-valley and spin-orbit splittings, as well as hydrostatic and biaxial strains. We will present multiple-period SiGe superlattices with large electric dipole moments and direct gaps at Γ yielded by this search.

[1]This work is supported through the Center for Inverse Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

Mayeul d'Avezac
NREL, Golden, Co

Date submitted: 26 Nov 2010

Electronic form version 1.4