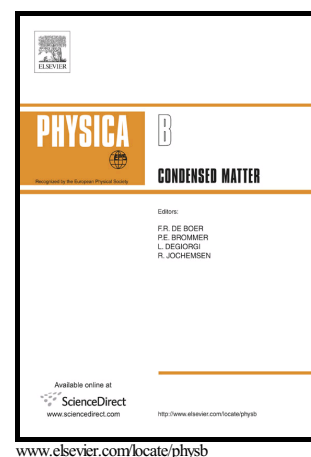


Unfolding and effective bandstructure calculations
as discrete real- and reciprocal-space operations

Timothy B. Boykin, Arvind Ajoy, Hesameddin
Ilatikhameneh, Michael Povolotskyi, Gerhard
Klimeck



PII: S0921-4526(16)30080-1
DOI: <http://dx.doi.org/10.1016/j.physb.2016.03.011>
Reference: PHYSB309398

To appear in: *Physica B: Physics of Condensed Matter*

Received date: 1 February 2016
Revised date: 4 March 2016
Accepted date: 5 March 2016

Cite this article as: Timothy B. Boykin, Arvind Ajoy, Hesameddin Ilatikhameneh, Michael Povolotskyi and Gerhard Klimeck, Unfolding and effective bandstructure calculations as discrete real- and reciprocal-space operations, *Physica B: Physics of Condensed Matter* <http://dx.doi.org/10.1016/j.physb.2016.03.011>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Unfolding and effective bandstructure calculations as discrete real- and reciprocal-space operations

Timothy B. Boykin^{a,*}, Arvind Ajoy^c, Hesameddin Ilatikhameneh^b, Michael Povolotskyi^b, and Gerhard Klimeck^b

^aDepartment of Electrical and Computer Engineering, The University of Alabama in Huntsville, Huntsville, Alabama 35899 USA

^bNetwork for Computational Nanotechnology, School of Electrical and Computer Engineering, Purdue University, West Lafayette, Indiana 47907 USA

^cSchool of Electrical and Computer Engineering, Cornell University, Ithaca, New York 14853 USA

*Corresponding author. boykin@ece.uah.edu

ABSTRACT

In recent years, alloy electronic structure calculations based on supercell Brillouin zone unfolding have become popular. There are a number of formulations of the method which on the surface might appear different. Here we show that a discrete real-space description, based on discrete Fourier transforms, is fully general. Furthermore, such an approach can more easily show the effects of alloy scattering. We present such a method for treating the random alloy problem. This treatment features straightforward mathematics and a transparent physical interpretation of the calculated effective (i.e., approximate) energy bands.

Keywords: unfolding; supercell; alloy

1. Introduction

Approximate concepts in physics are often the most difficult to articulate and quantify, but quantification is essential for it establishes the range of validity of the approximation. The alloy concept is one which is particularly easy to explain in qualitative terms but which can be problematic to quantify. Semiconductor alloys are of particular technological interest, being found in lasers and transistors incorporated into nearly all consumer and industrial electronic

Download English Version:

<https://daneshyari.com/en/article/8161795>

Download Persian Version:

<https://daneshyari.com/article/8161795>

[Daneshyari.com](https://daneshyari.com)