Multiband Tight-Binding Model for Strained and Bilayer Graphene from DFT Calculations

T. B. Boykin[a], M. Luisier[b], N. Kharche[c], X. Jiang[c], S. K. Nayak[c], A. Martini[d], and G. Klimeck[e]
[a]University of Alabama-Huntsville, [b]ETH Zurich, [c]Renssealer Polytechnic Institute, [d]University of California-Merced, [e]Purdue University
e-mail: boykin@ece.uah.edu

INTRODUCTION

The single π–orbital Wallace model[1] has been successfully used to model extended, perfectly flat graphene sheets, where the bands decouple into two non-interacting sets, the σ– and π–bands; the largely p_z-like π–bands are most relevant for transport. However, this model has significant limitations: artificial symmetries, and critically, no ability to model hydrogen-passivated nanoribbons (GNRs). Because experimental GNRs usually have passivated edges, the Wallace model[1] cannot simulate experiments. To remedy these problems we have recently developed a six-band $\{p,d\}$ model for the π–bands of flat graphene[2].

Real graphene structures, in contrast, generally have ripples and corrugations: Ishigami, et. al.[3] find that graphene on SiO_2 substrates at least partially conforms to the substrate, with local strains up to 1%. These ripples couple the σ– and π–bands, so that a proper approach for device modeling such as graphene FETs[4], must reproduce both sets of bands, accommodate in- and out-of-plane strains, and accurately model the long-range interactions of bilayer graphene. Also, the approach must be computationally efficient and suitable for interfacing with other semiconductor tight-binding models in order to simulate devices with graphene active regions.

MODEL AND RESULTS

We have developed a general-purpose multiband $\{s,p,d\}$ model for both the σ– and π–bands of graphene in order to treat these aspects of realistic graphene structures on substrates. Our model is parameterized to fit as closely as possible DFT calculations while still remaining computationally efficient. We concentrate on fitting the strain behavior of the most important band edges of graphene. Strain is accommodated by scaling the two-center integrals as $V = V_0 (d/d_0)^{-\eta} f(d/d_0)$ which is Harrison-like[5] at short ranges, yet accurately models the longer-range interactions in bilayer graphene. The function, f, is graphed in Fig. 1. The inset shows the strain region, where $f \approx 1$, while in the bilayer graphene region Harrison-type scaling is no longer valid and f is much smaller.

Figure 2 shows the behavior under planar uniaxial [10] strain of the M1 gap for our model and the reference DFT results to which it was fit. (The DFT-LDA gap at each strain was scaled by the ratio of the zero-strain gap as calculated by DFT-GW and DFT-LDA.) As reported in Fig. 2 the fit is good over a wide range of strain.

The importance of accommodating ripples is illustrated in Figs. 3 and 4. Figure 3 shows a GNR with ripples, with the ripples determined by molecular dynamics (MD) simulations using LAMMPS[6]. Figure 4 plots the transmission for this nanoribbon either flat (ballistic) or of varying lengths. The flat GNR exhibits the expected sharp step pattern, which degrades progressively as ripples are introduced and the structure becomes longer. This deterioration is explained by the increase in scattering as a function of the GNR length. It is expected that the apparent mobility of realistic GNR devices might be strongly limited by the ripple magnitude.

The suitability of our new scaling function for much longer range interactions is shown in Fig. 5 where we plot the bands of bilayer graphene. Figure 5 shows the expected small splitting in the bands for the bilayer material.

CONCLUSION

We have developed a multiband $\{s,p,d\}$ model so that with one single set of parameters both the σ– and π–bands of graphene, with and without strain, and in single-, bi-, and multi-layer structures can be accurately and efficiently reproduced. Our model successfully treats rippled graphene and it is therefore well suited for realistic graphene-based device simulations.

ACKNOWLEDGEMENT

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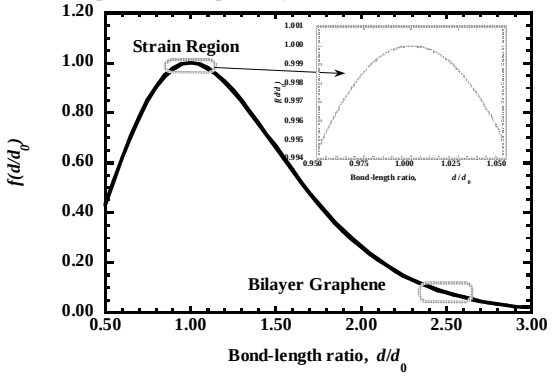

Fig. 1 Universal scaling function modulating Harrison-scaled two-center integrals. Inset: strain regiόn. The bilayer graphene region has much greater decay.

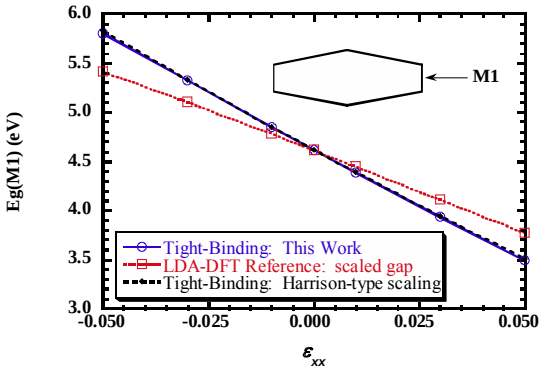

Fig. 2. M1 gap behavior under uniaxial [10] strain of our tight-binding model (both Harrison-type scaling and our new scaling function) and the scaled DFT-LDA reference results.

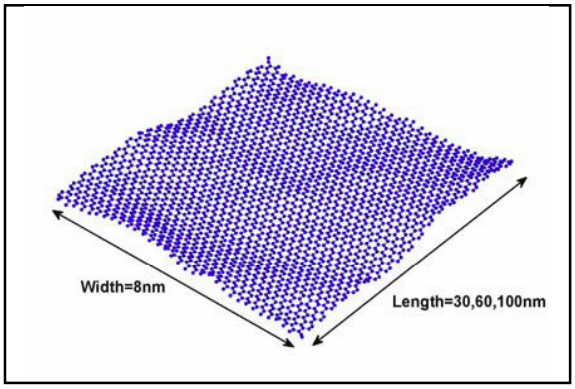

Fig. 3. GNR with ripples used for the transport simulations shown in Fig. 4. The ripples are introduced through MD simulations which relax the atom positions.

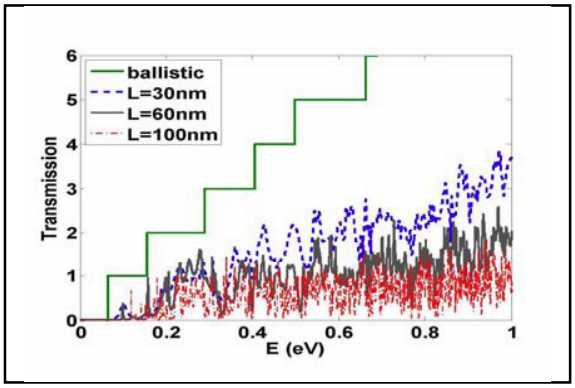

Fig. 4. Electron transmisssion through the GNR illustrated in Fig. 3. Ballistic results are for a perfectly flat GNR and show the expected stair-steps. The transmission progressively degrades with increasing length due to increased scattering.

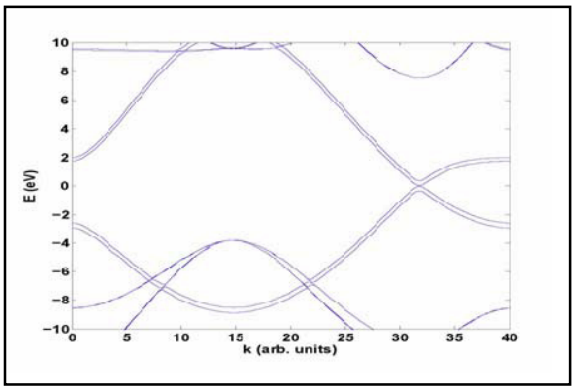

Fig. 5. Bands of bilayer graphene as calculated with our tight-binding model and new scaling function.