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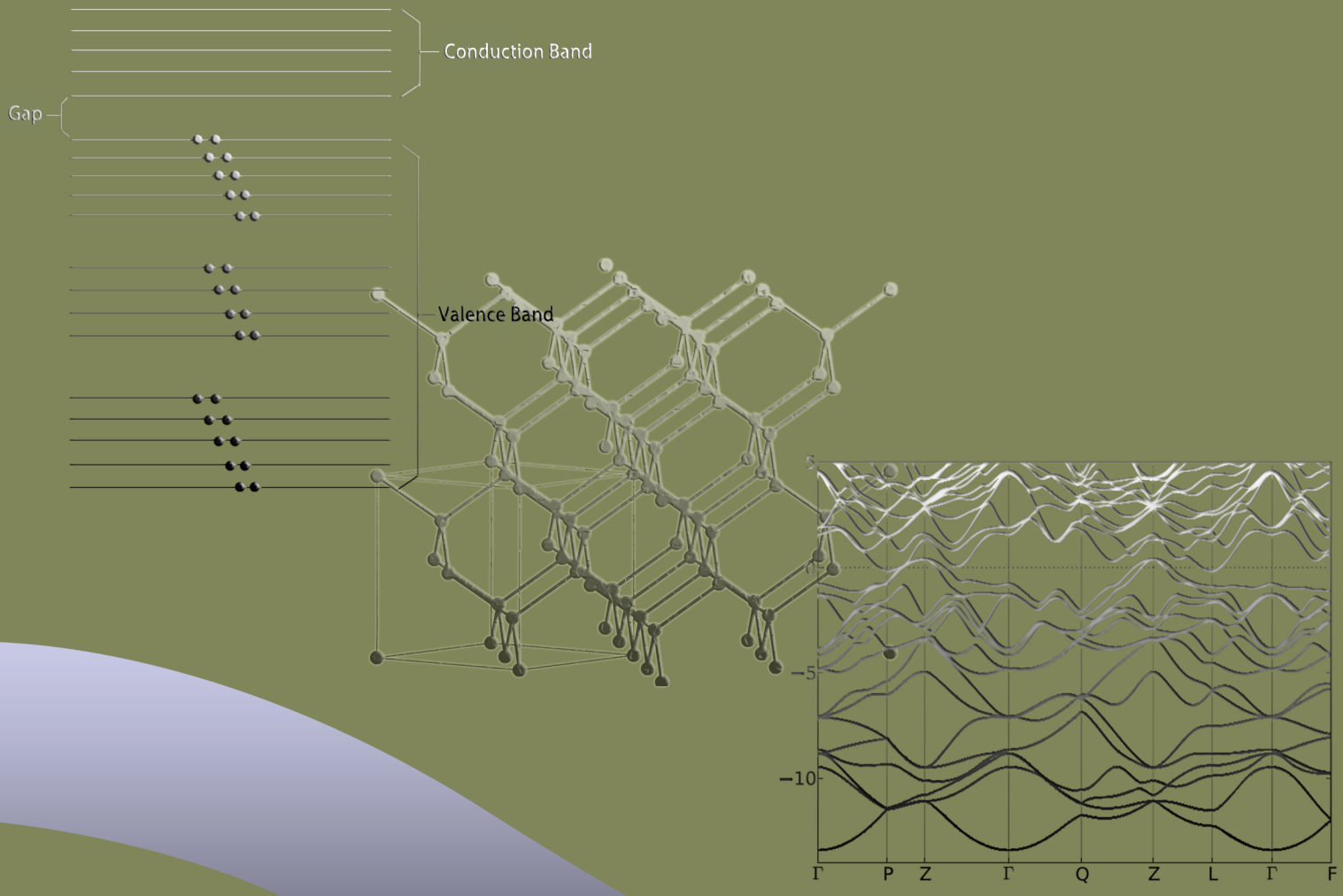
About Continuous Random Network Modeling



The continuous random network (CRN) model was proposed 70 years ago by Zachariasen [1] and is believed to be the counterpart of covalent amorphous materials as what the perfect crystal is to real crystalline materials, i.e. the ideal representation [2]. At first, it should be pointed out that although amorphous network possesses large amount of structure distortion compared to crystalline structure, there is physical restriction for the randomness, i.e. the local environment should be as close as possible to that of a crystal.

Typically, there were several methods to build up CRN, which is Wooten-Winer-Wearie (WWW) algorithm [3], molecule dynamics (MD) based algorithm [4, 5, 6, 7] and the activation-relaxation technique (ART) [8]. For detailed comparison between these methods, refer to Ref. [2, 9]. It should be pointed out that the WWW algorithm remains the basic approach for generating high-quality CRNs till today [2, 10]. For WWW approach, it fixes a list of topological bonds and then moves several of the local bonds topologically, and this way of changing the local structure is called bond transposition (see Ref. [2] Fig. 1 for illustration). After the structure changing, the overal force and energy will be calculated to evaluate whether to accept or reject the changing with the Metropolis acceptance probability [2]:

$$P = min[1, exp(\frac{E_b - E_f}{k_B T})] \tag{1-1}$$

The energy and force is calculated using the Keating potential:

$$E = \frac{3}{16}\frac{\alpha}{d^2}\sum_{\langle ij\rangle}(\mathbf{r}_{ij}\cdot\mathbf{r}_{ij} - d^2)^2 + \frac{3}{8}\frac{\beta}{d^2}\sum_{\langle jik\rangle}(\mathbf{r}_{ij}\cdot\mathbf{r}_{ik} + \frac{1}{3}d^2)^2 \tag{1-2}$$

where α and β are the bond-stretching and bond-bending force constant, which should be changed accordingly for different system (e.g. Si, Ge, GaAs, etc.) and d is the strain-free local bond length (e.g. the Si-Si bonding in the diamond structure). For Si, the theoretical value for α and β is $2.965eV$ and 0.285α, respectively [2] (Ref. [11] gives different value: $\alpha = 3.031eV$ and $\beta = 0.285\alpha$). For Ge, the theoretical value for α and β is $2.438eV$ and 0.16α, respectively.

Based on the WWW algorithm, there are quite a few improvement given in Ref. [2], and here we only focus on the random initial configuration. The original WWW algorithm starts from crystalline structure and then do the bond transposition until getting the final CRN, which is time consuming. The optimized method given in Ref. [2] first builds up a random framework and then follow the normal WWW algoritm, which can save a lot of time. The corresponding code can be found following the link: C-code for CRN modeling, by unpacking which we can obtain three folders - 'genran', 'example' and 'source'. The 'genran' folder contains the code needed to build up the initial random configuration, and there is included corresponding 'Makefile' for the convenience of compiling under Unix based computers (thus one can 'cd' into 'genran' and simply type 'make' in the command line to compile). After compiling, we can then execute the 'genran' file to obtain 'initial_configuration.dat' file which contains the initial random configuration of atoms. The main WWW algorithm based code can be found in 'source' directory, and also the 'Makefile' is included. Then we can copy

the created 'initial_configuration.dat' file from last step to the 'source' directory and then execute 'keating' file (the compiled binary file in 'source' directory) by adding the argument, i.e. './keating initial_configuration.dat'.

Another thing to mension is about the changing of parameters. To change the number of atoms in the simulated system, we can edit the 'genran.c' file (in 'genran' directory) and change the definition for 'N' from its original value to what we need. More importantly, the atom number should also be changed for the main WWW code, for which we can go to 'source' directory and edit the 'defs.h' file to change the value of 'N' to the same value that we changed it to in 'genran.c'. Also, in 'defs.h' file we can change temperature, equiblium local bond length, and force constant α and β.

The last thing to mention is that for each Keating simulation run, it is better to backup corresponding 'genran' folder (which contains the initial configuration) and also the 'defs.h' file (which contains all parameters used for the simulation) for later checking.

References

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