Visualization Techniques for Semiconductor Bandstructures

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Abstract

Visualization of semicondcutor bandstructures is accomplished in the 3-D Brillouin zone by using color rendering techniques to generate energy isosurfaces and color contour plots on crossectional planes. Combination of the various techniques offers an efficient way to analyze the data an get physical insight relevant for carrier transport. The visualization is performed on a Digital 5000 workstation using the Application Visualization System (AVS) graphics software.

I. Introduction

Advanced investigations of transport phenomena in semiconductors require a detailed knowledge of the energy bandstructure. This is particularly true when high energy effects are investigated, since available analytical formulations of the bandstructure are inaccurate or incomplete. For instance, some Monte Carlo applications suitable for the simulation of impact ionization and of other effects relevant for device reliability, implement algorithms with a full bandstructure for the evaluation of momentum space trajectories. We found that 3-D visualization of the bandstructure in momentum space is an important step for the understanding of the transport physics and for the development of optimization techniques for this type of Monte Carlo simulations. Since scattering rates are also closely related to the bandstructure, the same visualization techniques can be applied to analysis of the momentum dependence of scatterings.

We have experimented with a number of available visualization tools and we have found the Application Visualization System (AVS) software to be very suitable for these 3-D visualization problems. In the AVS environment, most of the applications are built by an interactive symbolic procedure, assembling an application network with modules available in a menu. Custom applications can be developed by writing additional modules using C language programming. An example of AVS application network we have used to visualize the bandstructure of silicon is shown in Fig. 1.

II. Visualization Approach

The approach which we found most effective to visualize energy bandstrutures is an animation of energy isosurfaces. We have built a Brilluoin zone and we display the isosurfaces in the cube which contains it. The slight redundancy of information which falls outside the zone helps in getting a visual appreciation of the connection between adjacent Brillouin zones. Since an isosurface only displays information for one energy value at a time, it is often necessary to combine this technique with others to get a more complete idea of the overall behavior. Several isosurfaces can be displayed at one time with the use of transparency and color coding, athough this may lead to extremely complicated images. This type of visualization is better suited to visualization of only the irreducible wedge of the Brillouin zone. On a full scale, we found very useful to combine energy isosurfaces with cross-sectional planes where a color contour plot of energy is represented. The isosurfaces are generated only on one side of the plane, which can be made to slide back and forth, and the intersections between the surfaces and the plane offer very helpful visual cues. The capability to perform rotations of the solid figure allows then the viewer to pinpoint any specific region of interest. An example of AVS application network we have used to visualize the bandstructure of silicon is shown in Fig. 1. The network represents actual subroutines which are assembled in a symbolic way. The bandstructure data is input through the branch beginning with the block *read field* while the Brillouin zone is constructed by the adjacent branch beginning with *read geom*. The image is displayed after the program runs through all the blocks, and the user can then interactively modify the image attributes, like orientation, size, color palette, lighting, to adjust the image, or can run again the program by simply modifying visualization parameters, like the value of energy isosurface, the position of the cross-sectional plane, or the data displayed in the given geometry (e.g. switch from bandstructure to scattering rates). The program can also be changed interactively, by breaking the connections in the network, and adding or subtracting modules. A large amount of information can be visualized at one time, since the isosurfaces can be color coded with another parameter (e.g. scattering rate) so that by scanning isosurfaces at different energies a 5-D space is represented.

We present here several examples of 3-D visualization for the silicon energy bandstructure. Figure 2a shows a view of a cross-sectional 100 plane for the first branch of the conduction band in the full Brilluoin zone. For the sake of reproduction, we use here a gray-scale palette, ranging from black (lowest energy) to light gray (highest energy). For color representation, we normally use the conventional rainbow coloring scheme, ranging from blue to red. It is easy to detect the four X-valleys situated on this plane in correspondence of the darkest regions. The same image for the second branch of the conduction band is shown in Fig. 4a. In both images, the energy isosurfaces are behind the cross-section. On the computer, the position of the plane can be moved interactively in real time by translation or rotation. Figures 2b, 3a,b and show the full isosurface configuration, at various energies, for he first conduction band branch, and Fig. 4b for the second branch. Figure 5 and 6 show results for the conduction band of gallium arsenide. The silicon-like X-valley isosurfaces can be easily identified by comparison with the previous images.

The data for the bandstructure were obtained by using an empirical pseudopotential approach. All the images are based on a cubic uniform mesh with 41 nodes on each side. The visualization was performed with AVS software on a Digital 5000 workstation and the images have produced on a Tektronix dye sublimation printer.

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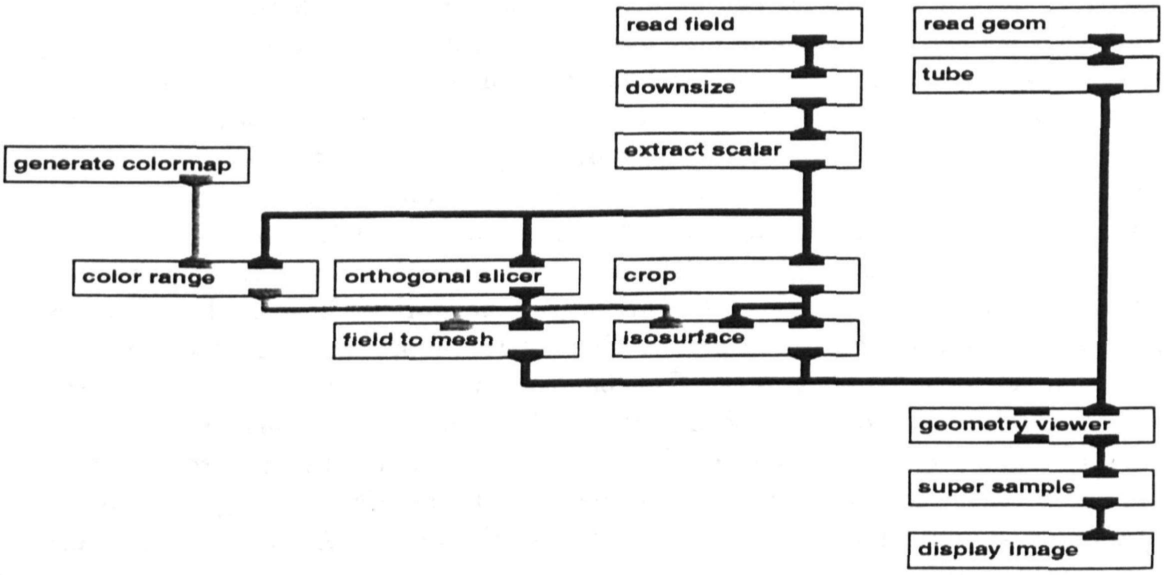

Figure 1. Simplified AVS network used for the visualization.

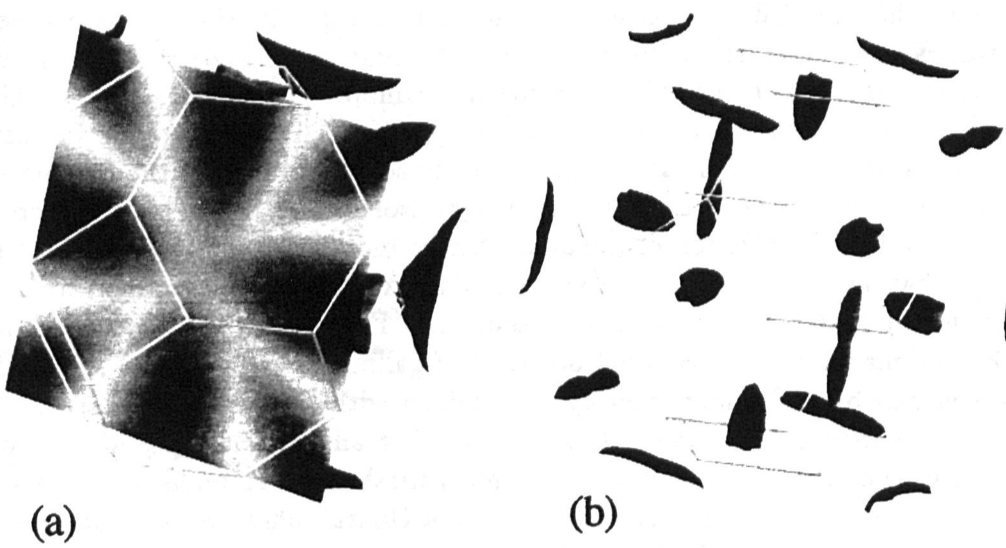

Figure 2. (a) Gray-scale contour plot of the first conduction band for silicon on the {100} plane; (b) Energy isosurfaces at $E = 0.2\ eV$.

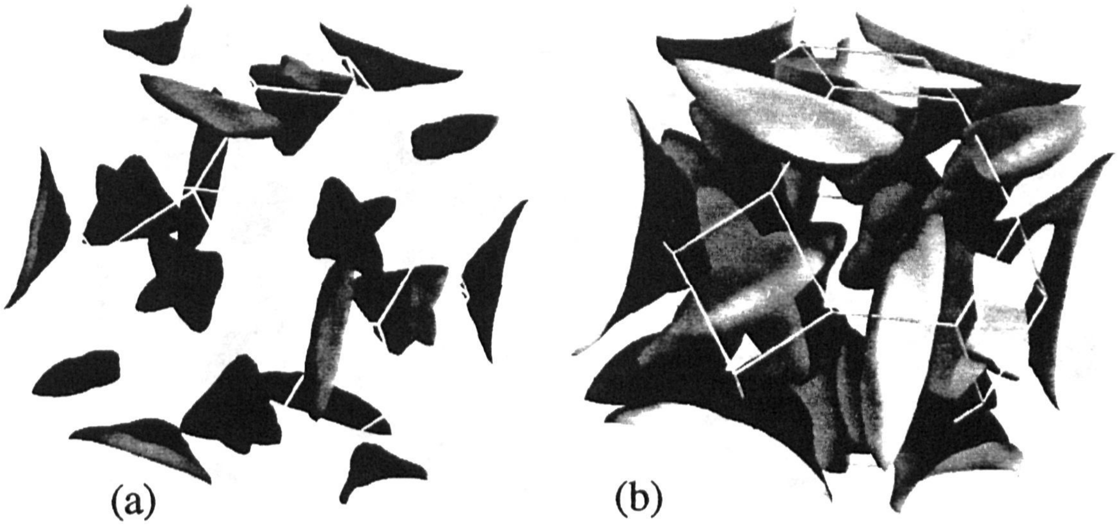

Figure 3. Energy isosurfaces of the first conduction band for silicon at (a) $E = 0.5\ eV$ and (b) $E = 1.5\ eV$.

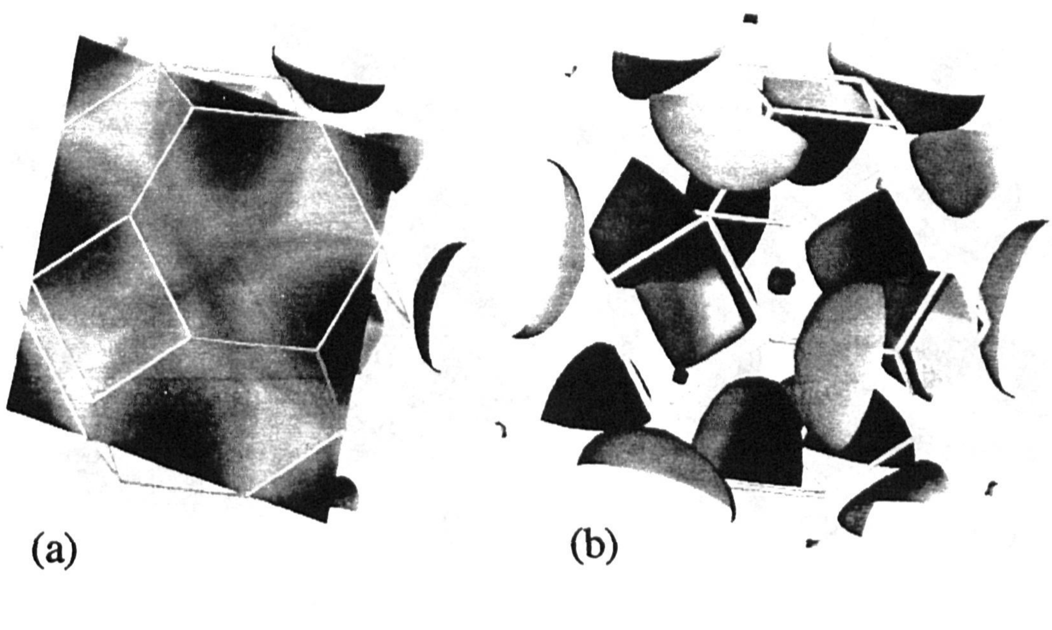

Figure 4. (a) Gray-scale contour plot of the second conduction band for silicon on the $\{100\}$ plane; (b) Energy isosurfaces at $E = 2.4\ eV$.

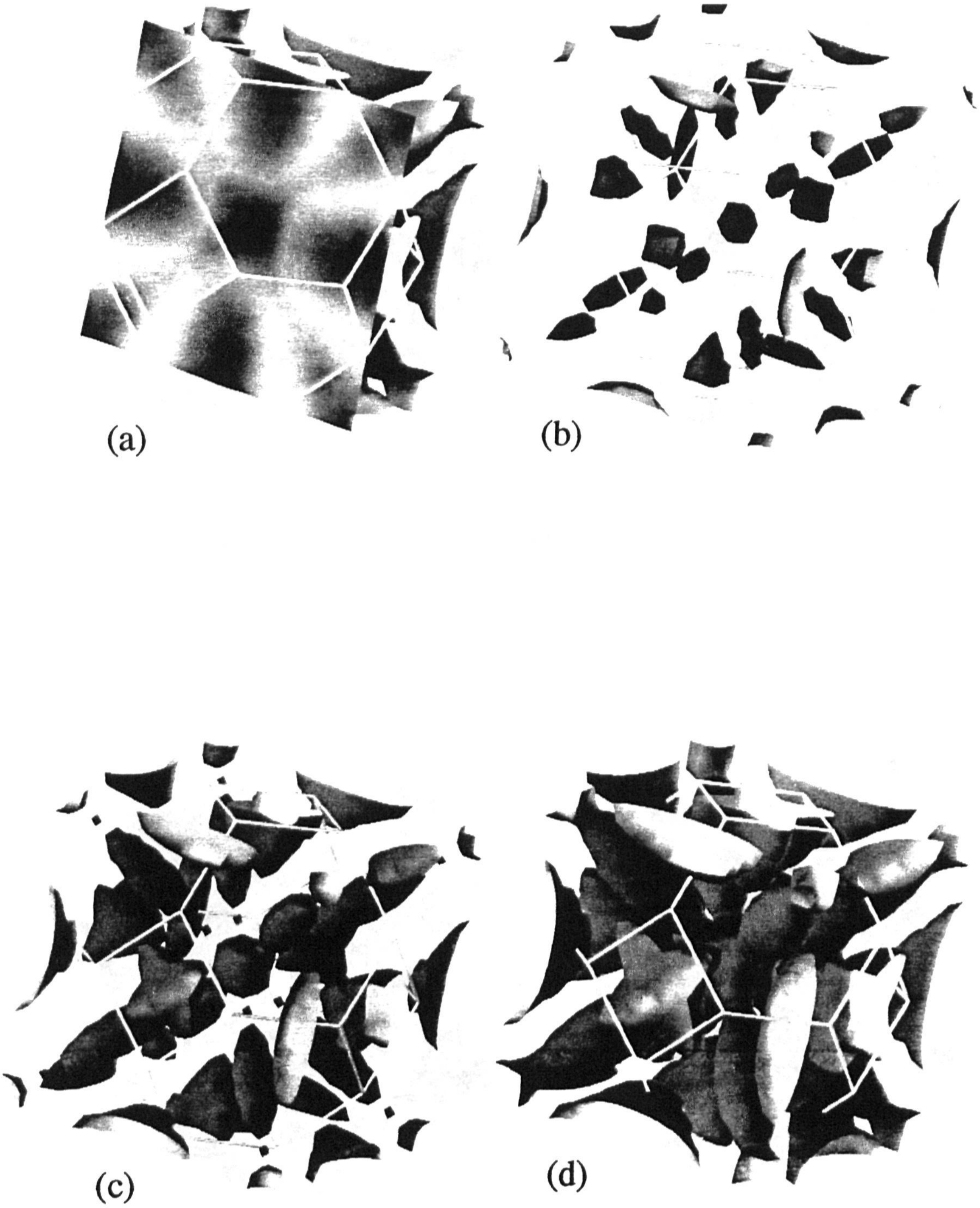

Figure 5. (a) Gray-scale contour plot of the conduction band for GaAs on the {100} plane; Energy isosurfaces at (b) $E = 0.75\ eV$; (c) $E = 1.1\ eV$; (d) $E = 1.5\ eV$.