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Citation	Journal of Applied Physics, 79(3), 1511-1514 https://doi.org/10.1063/1.360993
Issue Date	1996-02-01
Doc URL	https://hdl.handle.net/2115/5716
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Type	journal article
File Information	JAP79-3.pdf



Tunneling through a narrow-gap semiconductor with different conduction- and valence-band effective masses

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(Received 25 July 1995; accepted for publication 1 November 1995)

We have calculated tunneling conductance in metal–narrow-gap-semiconductor (NGS)–metal tunnel junctions. Flietner's two-band model is used to describe the dispersion relation within the energy gap in an isotropic NGS with different conduction- and valence-band edge effective masses. The results are compared with the tunneling conductance calculated by Kane's two-band model, which has been commonly used to describe the tunneling characteristics through the energy gap in semiconductors. These results propose that the tunneling conductance in the tunnel junctions in which a narrow gap semiconductor of largely different conduction- and valence-band effective masses is used as a tunneling barrier can exhibit quite a different behavior, especially in the region of the midgap, from the tunneling conductance described by Kane's two-band model. © 1996 American Institute of Physics. [S0021-8979(96)08203-3]

I. INTRODUCTION

Metal–semiconductor–metal tunnel structures have been mainly studied in relation to Josephson junctions, in which the metal electrodes are superconductors.¹ These studies have been motivated by the possibility of high-frequency applications such as detectors, superconducting quantum interference device (SQUID) magnetometers, etc.,² due to the relatively low dielectric constant of the semiconductors. However, up to now tunnel structures in which normal metals are used as electrodes have scarcely been reported³ although these systems with a semiconductor barrier are intrinsically interesting with regard to the physics of tunneling. Narrow-gap semiconductors (NGS) are especially good candidates for the tunneling barrier, since a small energy gap leads to coupling of conduction and valence bands, namely, a nonparabolic dispersion relation, which can be described by a small and energy-dependent effective mass.⁴ In metal–NGS–metal tunnel structures, the small forbidden gap of a semiconductor consists of a tunnel barrier and therefore we expect a variety of tunneling conductance which reflects the nonparabolic dispersion relation even with a small applied voltage. This interest is based upon the fact that the energy dependence of the decay constant k in tunneling electrons can be described by the dispersion relation in the forbidden gap of the semiconductor.

On the other hand, much attention has been paid recently to mechanisms for the occurrence of negative differential conductance in a single-barrier structure, such as tunneling below midgap⁵ or interband tunneling.⁶ Of these, tunneling below midgap has been usually explained by Kane's two-band model (one-parameter model) as the simplest analytic expression.⁴ In this model, the origin of negative differential conductance in single-barrier tunneling can be ascribed to its energy-wave vector dispersion relation in the energy gap, in which the wave vector shows the maximum toward the mid-

gap and is symmetrical with respect to the midgap. That is, the tunneling probability is higher for tunneling electrons which have energy close to the valence-band edge and the imaginary wave vector of tunneling electrons increases as they approach the midgap of the tunneling barrier from near the valence-band edge. Therefore, as the applied bias voltage is increased, the tunneling conductance decreases below the midgap, and leads to a negative differential conductance; however, it is important to note that the above explanation depends strongly upon the adopted model. Kane's model can continue the conduction and valence bands by the $E-k$ curve analytically only when the conduction- and valence-band edge effective masses are exactly the same. Thus, Kane's model can only be applied to semiconductors that have exactly the same conduction- and valence-band edge effective masses. Little attention has been paid to this fact in analyzing the tunneling through a semiconductor barrier. It should be particularly noted that both effective masses are usually not the same in most semiconductors. Therefore, for the analysis of tunneling through a variety of NGS, the formulation of a tunneling equation using a more generally applicable two-band model, in which the different conduction- and valence-band edge effective masses are taken into account, is needed.

Flietner proposed a model for the dispersion relation in the energy gap under the assumption that the conduction- and valence-band edge masses are different (two parameter model).⁷ In this model, analytic continuation between two bands whose band edge effective masses are different can be successfully carried out by an asymmetric dispersion relation. By using this model, he successfully explained the experimental results about the surface states in the metal–semiconductor contacts.

Since it is well known that the tunneling characteristics are quite sensitive to the adopted model, it is interesting to investigate how the tunneling conductance can be affected by introducing the effect of the different effective masses of the conduction and valence bands for the dispersion relation of NGS as a tunneling barrier; however, as far as we know it

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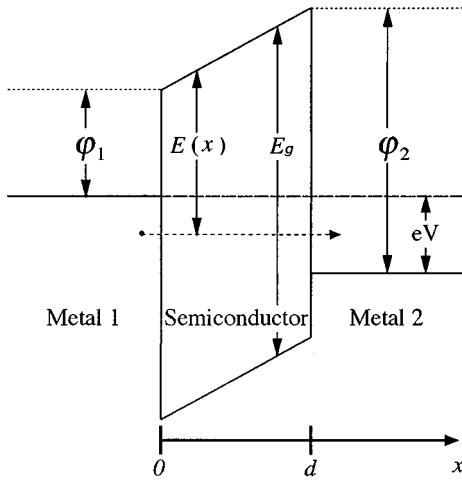


FIG. 1. Schematic energy band diagram in a metal–narrow-gap–semiconductor–metal tunnel junction. Trapezoidal barrier is assumed for a semiconductor tunneling barrier. Metal 1 is negatively biased to metal 2 by eV .

seems that there have been very few previous studies, whether experimental or theoretical, on how such an asymmetric dispersion relation within the energy gap caused by the different conduction- and valence-band effective masses leads to tunneling characteristics. We have thus performed the calculations of the tunneling conductance in metal–NGS–metal tunnel structures by introducing Flietner’s model for the more general dispersion relation of NGS in the tunnel equation and the comparison with the result calculated by Kane’s model. We predict how the difference of the conduction- and valence-band effective masses can affect the tunneling characteristics through NGS.

II. FORMULATION

We consider a trapezoidal model shown in Fig. 1 and ignore surface effects such as surface levels, accumulation, or inversion layer. In this model two metals are separated by a NGS thin-film tunnel barrier. We start with the general expression for the tunnelling current density,⁸

$$J(V) = \frac{e}{2\pi^2\hbar} \int \int \int dE d^2k_t \times [f(E) - f(E + eV)] D(E, k_t, x). \quad (1)$$

Here D is the transmission factor and the Fermi function factors $[f(E) - f(E + eV)]$ guarantee that the initial state is occupied and that the final state is empty. The x coordinate dependence of D is due to the applied potential. The tunneling electron energy E and the transverse momentum k_t conservation laws are explicit in Eq. (1) because of the use of a common value of E and k_t for all regions of the tunnel structure.

From the above equation we can obtain the below equation following the procedure of Kurtin and co-workers,³

$$J(V) = \frac{e}{2\pi\hbar} \int_0^V dE \times \exp\left(\frac{-2d}{\varphi_1 - \varphi_2 + eV} \int_{-(\varphi_1 - E)}^{-(\varphi_2 - eV - E)} k(\epsilon) d\epsilon\right) \times \left(\int_{-(\varphi_1 - E)}^{-(\varphi_2 - eV - E)} \frac{dk(\epsilon) d\epsilon}{\varphi_1 - \varphi_2 + eV}\right)^{-1}. \quad (2)$$

We take the conduction-band edge in NGS as the origin of the energy. In the above equation the transmission factor is expressed by the WKB approximation. The integral of the transverse wave vector is based on the physical assumption that the tunneling probability decreases rapidly with the increase of the transverse wave vector and is done by the method of steepest descents.⁹ The Fermi function factors have disappeared by $T=0$ K approximation.

The tunneling experiments in metal–NGS–metal structures are usually carried out at below liquid-helium temperatures to eliminate thermionic currents over the barrier whenever possible, so it is sufficient to consider this equation within the limits of $T \sim 0$ K. Therefore, Eq. (2) is the basis for an analysis of the tunneling characteristics near 0 K through the semiconductor tunnel barrier which has an arbitrary $E-k$ dispersion relation. In the formalism in which the dispersion relation is incorporated, it is clear that a tunneling electron has a different wave vector dependent upon the tunneling electron energy.

As the dispersion relation for the energy gap in NGS, Flietner’s model is used, in which the different conduction- and valence-band edge effective masses are incorporated. To apply it in the tunnel equation (2), Flietner’s dispersion relation had to be rewritten in the following way:

$$\frac{\hbar^2 k^2}{2m_c^*} = \epsilon \left(1 + \frac{\epsilon}{E_g}\right) \left(1 + \alpha \frac{\epsilon}{E_g}\right)^{-2}, \quad (3)$$

where

$$\alpha = 1 - \sqrt{m_c^*/m_v^*}. \quad (4)$$

Here m_c^* and m_v^* are the effective masses at the conduction- and the valence-band edges, respectively. We note that Flietner’s model can be reduced to Kane’s model for the case of $\alpha=0$ ($m_c^* = m_v^*$). We cannot calculate the above tunnel equation (2) analytically except in the case of $\alpha=0$, so we have performed the calculation numerically.

III. RESULTS AND DISCUSSION

First dispersion relation curves calculated using Flietner’s two-band model are given in Fig. 2. As typical values in NGS, we take $E_g=300$ meV for the energy gap, $m_c^*=0.03$ for the conduction-band edge effective mass and $m_c^*/m_v^* = 0.1, 1.0, 2.0$ for the conduction- and valence-band edge effective mass ratio, respectively. Of these, we note that $m_c^*/m_v^* = 1.0$ corresponds to Kane’s model. Figure 2 shows that the calculated curves that use the different conduction- and valence-band edge effective mass ratios ($m_c^*/m_v^* = 0.1, 2.0$) calculated with Flietner’s model are quite different compared to the curve calculated with Kane’s model. Therefore,

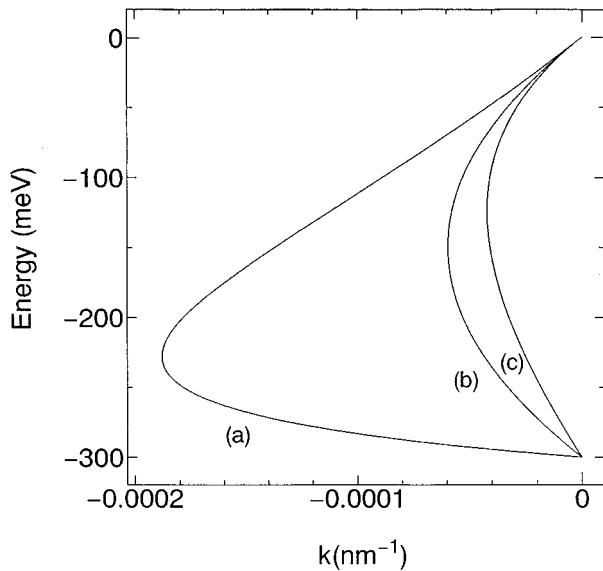


FIG. 2. $E-k$ dispersion relations calculated by Flietner's model. $E_g=300.0$ meV and $m_c^* = 0.03$. m_c/m_v is (a) 0.1, (b) 1.0, (c) 2.0, respectively. $m_c^*/m_v^* = 1.0$ corresponds to Kane's model.

we expect that such differences in the $E-k$ relations will lead to quite different tunneling characteristics from those obtained by Kane's model. It should be emphasized that in Flietner's model the coupling effect between conduction and valence bands cannot always be the strongest in the middle of the energy gap unless the conduction- and valence-band edge effective masses are exactly the same. We calculate tunneling conductance $dJ(V)/dV$ to clarify the difference in the tunneling characteristics derived from the asymmetric dispersion relation below.

Figure 3 shows the tunneling conductance in the case that the Fermi energy is located near the valence-band edge ($\varphi_{1,2}=280.0$ meV) in NGS. In the case of $m_c^*/m_v^* = 0.1$ the tunneling conductance shows a narrower peak and stronger saturation after the conductance minimum compared with that calculated from the Kane model. On the other hand, in the case that the valence-band edge effective mass m_v^* is smaller, the conductance peak becomes broader and the saturation in the conductance is weaker than that calculated by Kane's model. Thus, we find that the shape of the tunneling conductance exhibits very different behavior depending upon the different effective mass ratio. This result predicts that the consideration for the difference of the effective mass is important in the analysis of the tunneling characteristics through a NGS of different conduction- and valence-band effective masses. Such a characteristic tunneling conductance has rarely been observed before. We observed a narrow width conductance peak at 0 meV and a strong saturation of the conductance in Au-Sb₂Te₃-Al tunnel junctions, in which Sb₂Te₃ is a V-VI narrow-gap semiconductor.¹⁰

Next, we show the tunneling conductance in the case where the Fermi energy locates deep in the energy gap ($\varphi_{1,2}=180.0$ meV) in Fig. 4. We see that the conductance calculated from Kane's model shows a clear negative differential conductance in this bias region. On the other hand, the introduction of the different effective masses, m_c^* and m_v^* in

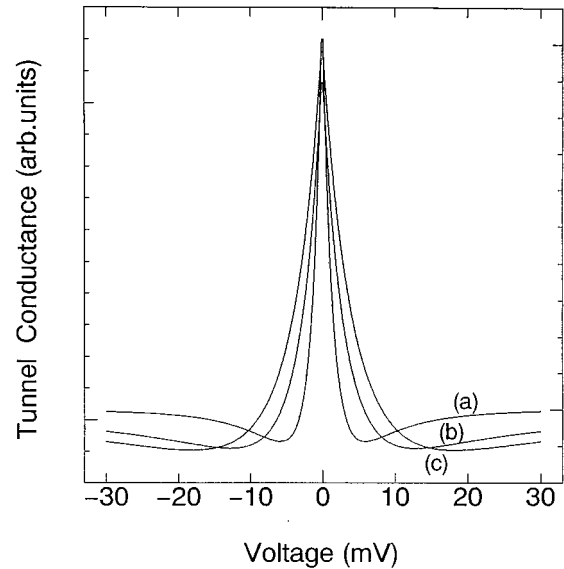


FIG. 3. Tunneling conductance in a metal-NGS-metal tunnel junction calculated by Flietner's model in the case that the Fermi level locates near the valence-band edge. $E_g=300.0$ meV, $m_c^* = 0.03$, $\varphi_{1,2}=280.0$ meV, and $d=40.0$ nm. m_c^*/m_v^* is (a) 0.1, (b) 1.0, (c) 2.0, respectively. Note that a narrower conductance peak and a stronger saturation after the conductance minimum in the case of $m_c^*/m_v^* = 0.1$.

Flietner's model leads to the similar negative conductance or quite different flat conductance exactly in the same bias region, depending on the band-edge effective mass ratio. From Figs. 2 and 4 we expect the appearance of negative differential conductance or flat shape conductance in a wider energy region of the energy gap than that we would expect from Kane's model. Moreover, the results propose that the shape of the tunneling characteristics near the midgap region is

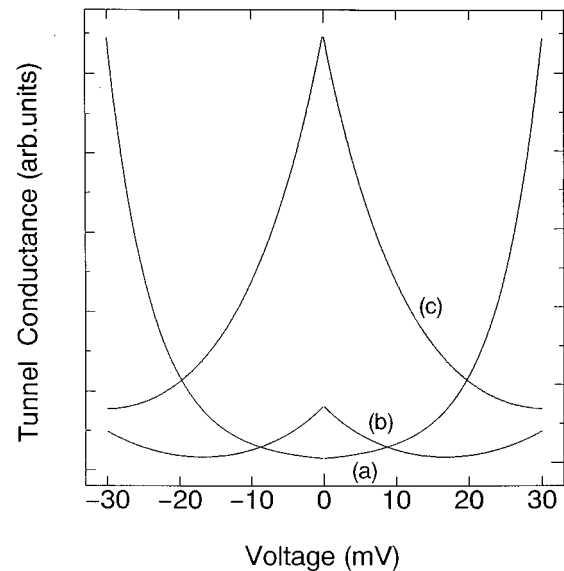


FIG. 4. Tunneling conductance in a metal-NGS-metal tunnel junction calculated by Flietner's model in the case that the Fermi level locates deep in the energy gap. $\varphi_{1,2}=180.0$ meV. The other parameters are the same as those in Fig. 3. Note that each curve shows quite different tunneling characteristics.

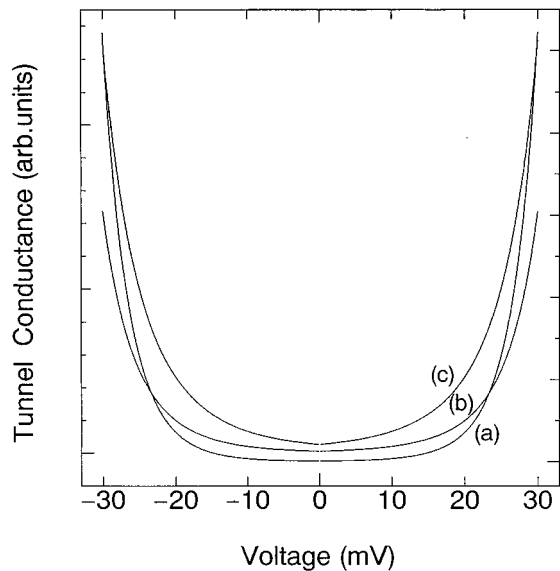


FIG. 5. Tunneling conductance in a metal-NGS-metal tunnel junction calculated by Flietner's model in the case that the Fermi level locates at near the conduction-band edge. $\varphi_{1,2}=80.0$ meV. The other parameters are the same as those in Fig. 3.

more dependent upon the conduction- and valence-band edge effective mass ratio than that of the tunneling characteristics in the energy regions near the valence-band edge (and the conduction-band edge as shown later). The drastic change of the tunneling conductance dependent upon the effective mass ratio in the vicinity of the midgap region would propose that it is quite important to use the two-band formula considering the difference of the conduction- and valence-band effective masses such as Flietner's model, particularly in the energy region.

Again we should pay attention to the fact that the maximum of the wave vector in the energy gap always locates at just the midgap in the case of Kane's model. That is, in this model a negative differential conductance can always be observed below the middle of the energy gap. Certainly, it seems that the previous studies^{11,12} of the tunneling characteristics in the energy region toward the midgap from the valence-band edge through a semiconductor barrier have often used Kane's model which includes only a single band edge effective mass without paying attention to the difference between the conduction- and the valence-band edge effective masses. It should be remembered that Kane's model is completely valid only in the case of $m_c^* = m_v^*$. Our analysis demonstrates conclusively that the consideration for the difference of the effective masses is essential also in this energy region in the analysis of the tunneling characteristics. Therefore, we believe that an analysis which takes into account the different effective masses is necessary.

Figure 5 shows the tunneling conductance in the case where the Fermi energy locates near the conduction band ($\varphi_{1,2}=80.0$ meV). The circumstance where the Fermi level of

the metals locates at the upper half of the energy gap is well known in a metal-metal-oxide-metal tunnel junction, in which metal oxide has a large energy gap ($\geq \sim 5.0$ eV). From this figure we can recognize that the change of the conductance becomes larger near the zero bias voltage as m_c^*/m_v^* changes from 0.1 to 2.0 and that in the case of $m_c^*/m_v^* = 0.1$ the tunnel conductance shows a flat shape in the wider energy range and a sharp rising. Therefore, we can predict that the difference of the effective masses m_c^* and m_v^* has to be considered also in this energy region.

IV. CONCLUSION

We have proposed and analyzed the tunneling conductance in metal-NGS-metal tunnel junctions by using Flietner's model in which the different conduction- and valence-band edge effective masses are included. The results are compared with the results by Kane's commonly used two-band model. Such analysis have almost not been carried out on both the theoretical and experimental sides before. These results propose that the tunneling conductance in the junctions in which a NGS of largely different conduction- and valence-band effective masses is used as a tunneling barrier leads to a different tunneling conductance behaviour from Kane's two-band model, especially in the vicinity of midgap region. As the effective masses of the conduction and valence bands in semiconductors are usually different, we believe that the different effective masses of the conduction and valence bands should necessarily be included in the two-band analysis for tunneling through a narrow-gap semiconductor and, therefore, that the use of Flietner's two-band model for an analysis of tunneling conductance in a metal-NGS-metal tunnel junction could bring us more accurate knowledge for tunneling through narrow-gap semiconductors. For the observation of the phenomena presented in this article we hope tunneling experiments shall be carried out in tunnel junctions in which a narrow-gap semiconductor of a largely different effective masses m_c^* and m_v^* such as InSb is used as a tunneling barrier, together with the suitable metal electrodes.

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