

Hole-Initiated Impact Ionization and Split-off Band in Ge, Si, GaAs, InAs, and InGaAs

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1. Introduction

It is now widely recognized that the details of the band structure are essential ingredients for the evaluation of the correct impact ionization rates in semiconductors. In particular, a satisfactory agreement between experiments and theory for electron-initiated impact ionization in Si has been recently reached and this process is now well understood.[1]

In most cases, however, empirical local pseudopotentials without spin-orbit interaction are commonly employed to calculate the band structure used in the calculation of *ab-initio* impact ionization rates.[2, 3, 4] The justification for doing so rests mainly on the speculation that the differences among the band structures obtained from local or nonlocal pseudopotentials, with or without spin-orbit interaction, are negligibly small compared to the energy scales involved in the ionization transitions, which are necessarily larger than the semiconductor band-gap. This is true at least partially, since these various approximations result in calculated band structures which exhibit very similar energies at symmetry k -points in the first Brillouin Zone (BZ), and differ significantly only as far as the split-off valence band is concerned. Its energy splitting, Δ , due to spin-orbit interaction is at most a few hundred meV, which is much smaller than the band-gap energy (see Table 1) in most cases, InAs being a notable exception. Therefore, it appears that the spin-orbit splitting could be safely ignored for the calculation of *ab-initio* rates of impact ionization in many semiconductors.

In this work, we investigate the correctness of this assumption by computing the hole-initiated impact ionization rates employing two different band structures, using nonlocal pseudopotentials with spin-orbit interaction or using local pseudopotentials and ignoring the spin-orbit splitting in the valence band. We demonstrate that the speculation described above is, in general, not true for *hole-initiated* impact ionization: The spin-orbit splitting

| semiconductor | split-off Δ (eV) | band gap E_g (eV) |
|---|-------------------------|---------------------|
| Si | 0.04 | 1.105 |
| Ge | 0.30 | 0.664 |
| GaAs | 0.33 | 1.420 |
| InAs | 0.38 | 0.356 |
| $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ | 0.36 | 0.727 |

Table 1: Spin-orbit energy splitting, Δ , and band-gap energy, E_g , employed in this work for various semiconductors.

is crucial to computing the correct rates for hole-initiated impact ionization. In addition, the matrix elements also play a significant role in direct narrow-gap materials such as InAs and $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$.

The present paper is organized as follows: In Section 2, the calculation scheme of *ab-initio* ionization rates is briefly summarized. The results of the calculation and a discussion are presented in Section 3. Finally, conclusions of this work are given in Section 4.

2. Calculation Scheme

The detailed calculation scheme of *ab-initio* impact ionization rates has been already presented in detail in many previous publications.[1, 2, 3, 4, 5] Therefore, only the basic ideas are given here.

The band structures for Ge, Si, GaAs, InAs, and $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ are obtained from local pseudopotentials [6] and nonlocal pseudopotentials with spin-orbit interaction [7]. The energy splitting Δ due to spin-orbit interaction at the Γ -point in the valence band is summarized in Table 1 for each material. The hole-initiated impact ionization rates are computed for these two different band structures using Fermi's golden rule. The band structure in the irreducible wedge (IW) of the first BZ is discretized with a cubic mesh of spacing $0.1 (2\pi/a)$, where a is the

lattice constant. The band-structure information (energies and pseudo wave-functions) at each \mathbf{k} -point outside the IW is extracted, during the computation of ionization rates, by applying the symmetry transformation from the corresponding \mathbf{k} -point inside the IW.[2, 4] The matrix elements for the ionization transition are evaluated for both the direct and exchange processes including *Umklapp* processes. Dielectric screening is assumed to be static, as already discussed in Ref. [1], so that the static dielectric function ($\omega = 0$) is employed.

3. Results and Discussion

As we have pointed out before,[1] electron-initiated impact ionization rates for *indirect* gap materials[8] are predominantly controlled by the density of states, not by the matrix elements, whereas for *direct* gap materials, both the matrix elements and the density of states play a crucial role in determining the scattering rates. Therefore, we shall discuss separately our results for indirect and direct gap materials.

Indirect-Gap Semiconductors

Hole-initiated impact ionization rates for Si, Ge, and GaAs obtained from the two different band structures (nonlocal with spin-orbit and local pseudopotentials without spin-orbit interaction) are shown in Fig. 1. With the notable exception of Si, the difference between the two results is remarkable: The overall energy dependence of the ionization rates depends dramatically on whether the spin-orbit interaction is taken into account. The densities of states in the valence bands under the two approximations are also plotted in Fig. 1. Notice that the first peak in the density of states obtained using local pseudopotentials and no spin-orbit interaction is shifted roughly by an amount equal to the energy splitting Δ . This shift is responsible for the difference seen in the hole-initiated ionization rates, as explained below.

According to the formula derived before,[9] the impact ionization rate $w_{ii}(\varepsilon_1)$ for holes with energy ε_1 is approximately given by the convolution of the density of states:

$$w_{ii}(\varepsilon_1) \approx C_{ii} \int_0^\infty d\varepsilon \rho_v(\varepsilon) \rho_v(\beta - \varepsilon), \quad (1)$$

where C_{ii} is a constant (related to the averaged matrix element of the ionization transitions) and ρ_v is the density of states for the valence bands. β is approximately a linear function of ε_1 :

$$\beta \approx \xi(\varepsilon_1 - \varepsilon_{th}), \quad (2)$$

with $\xi \approx 0.5$. Here, ε_{th} is the ionization threshold energy. Equation (1) implies that the ionization rate is determined by the density of states at low energy, since the upper integration limit of Eq. (1) extends only to β given by Eq. (2). This is consistent with the fact that the rate of impact ionization is mostly controlled by the joint density of states for the secondary carriers (two holes and

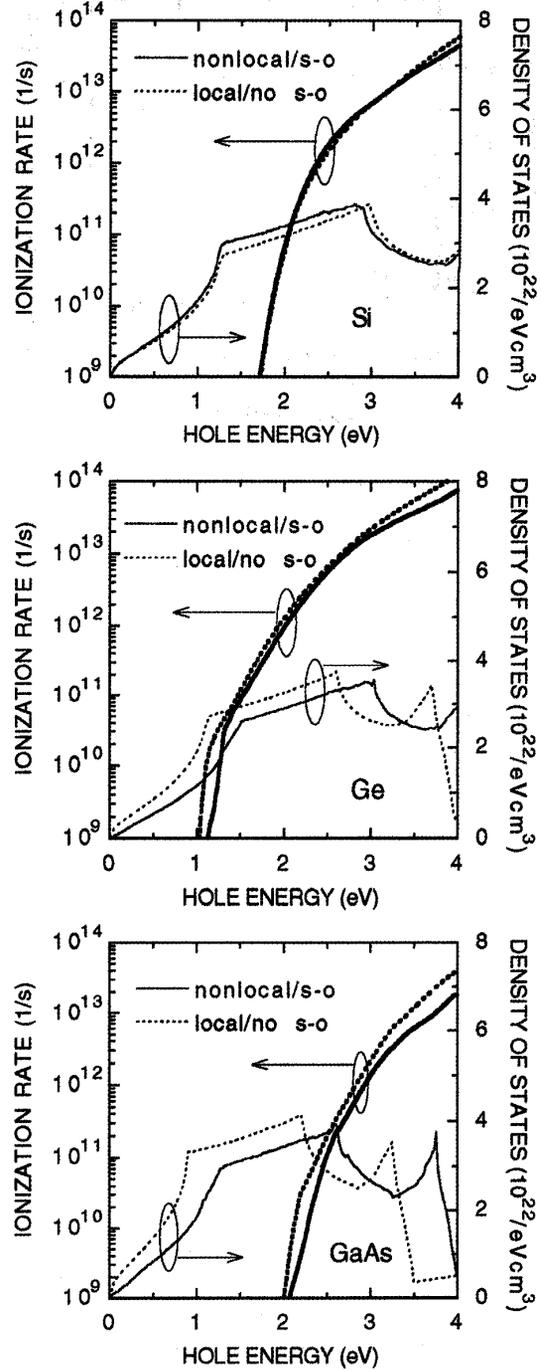


Figure 1: Calculated *ab-initio* rates for hole-initiated impact ionization (thick lines with left-scale) and density of states (thin lines with right-scale) in the valence band of Si, Ge, and GaAs. The solid and dotted lines represent, respectively, the results obtained using nonlocal and local pseudopotentials, with and without spin-orbit interaction, respectively

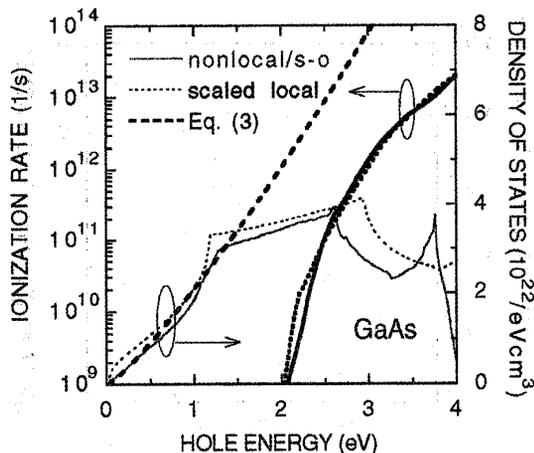


Figure 2: Scaled density of states (thin dotted line) and the density of states obtained from nonlocal pseudopotentials with spin-orbit interaction (thin solid line) in GaAs. The thick dashed line represents the density of states approximated by Eq. (3) with $s = 1.2$. The thick dotted line is the ionization rate calculated from Eq. (4) with $\alpha = 0.75$, whereas the thick solid line is the ionization rate using nonlocal pseudopotentials with spin-orbit.

one electron in this case), whose final states are close to the band edges. Thus, the detailed structure of the density of states at low energies critically affects the energy dependence of the ionization rate. In the case of GaAs, β is roughly equal to 1.2 eV for primary holes of $\varepsilon_1 = 4$ eV. Therefore, the hole-initiated ionization rate for GaAs is determined by the density of states of the valence bands in energy regions up to the first peak (≈ 1.2 eV) in Fig. 1.

In order to differentiate the roles played by the Coulomb matrix element and by the spin-orbit interaction, it is instructive to employ Eq. (1) and attempt to reproduce the *correct* ionization rate by taking into account only the energy splitting due to the spin-orbit interaction. The energy dependence of the density of states obtained using the two different band structures is similar. Thus, by simply scaling the hole energy as $\varepsilon \rightarrow \alpha\varepsilon$, we can transform the local-pseudopotential/no-spin-orbit density of states to a form similar to the density of states obtained using the other band structure. This scaled density of states for GaAs ($\alpha = 0.75$) is plotted in Fig. 2 along with the density of states obtained from nonlocal pseudopotential with spin-orbit interaction. We then assume that the density of states is proportional to hole energy raised to some power s ;

$$\rho_v(\varepsilon) = A_v \varepsilon^s. \quad (3)$$

Employing Eq. (1), the hole ionization rate $w_{ii}^{\text{scaled}}(\varepsilon_1)$ for the *scaled* density of states is now related to the ionization rate obtained using local pseudopotentials and no spin-orbit coupling, $w_{ii}^{\text{local}}(\varepsilon_1)$, by:

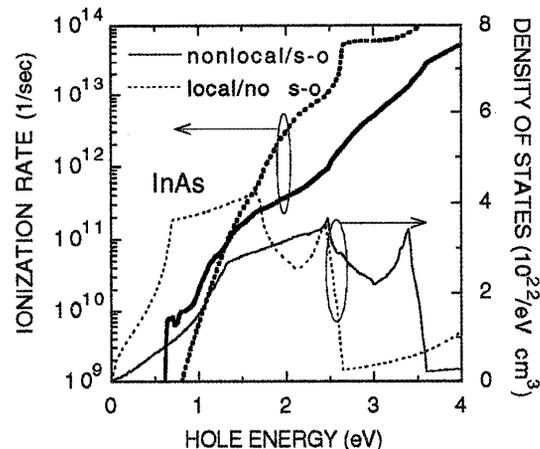
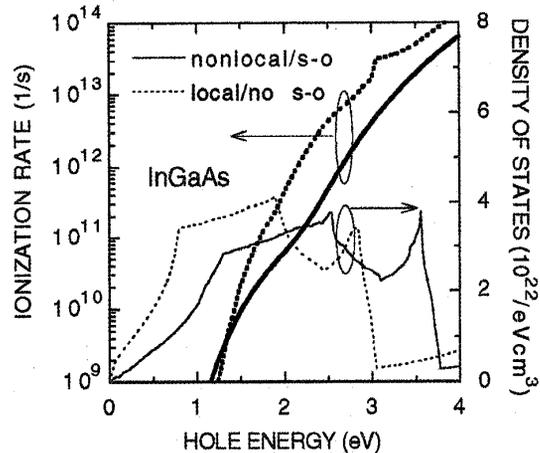


Figure 3: Hole-initiated impact ionization rates (thick lines with left-scale) and the density of states (thin lines with right-scale) of the valence bands in $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ and InAs. The solid and dotted lines represent, respectively, the results of nonlocal and local pseudopotentials, with and without the spin-orbit interaction.

$$w_{ii}^{\text{scaled}}(\varepsilon_1) = \alpha^{2s} w_{ii}^{\text{local}}(\varepsilon_1). \quad (4)$$

The *scaled* ionization rate obtained from Eq. (4) is plotted in Fig. 2. The exponent s assumed here for the energy dependence of the density of states is $s = 1.2$. The agreement between the two ionization rates (nonlocal with spin-orbit and *scaled, local* without spin-orbit) is excellent. This substantiates the idea that impact ionization is a *low-energy* process, in the sense that the density of low-energy recoil/secondary states determines the energy dependence of the ionization rates.

Direct-Gap Semiconductors

The situation is much more complicated for *direct* gap materials. Results of calculations for $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ and InAs are summarized in Fig. 3. The difference in the density of states between the results obtained using

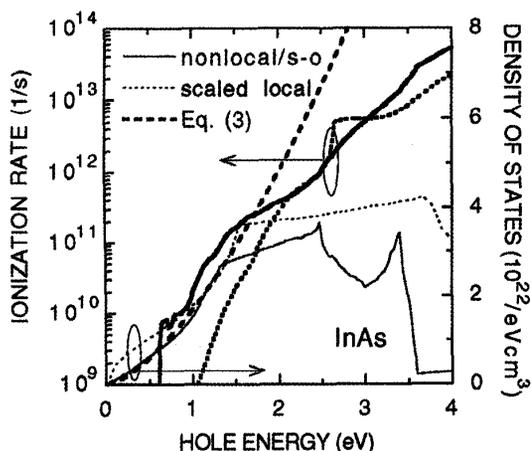


Figure 4: Scaled density of states (thin dotted line) and the density of states obtained from nonlocal pseudopotentials and spin-orbit coupling (thin solid line) in InAs. The thick dashed line represents the density of states approximated by Eq. (3) with $s = 1.5$. The thick dotted line is the ionization rate calculated from Eq. (4) with $\alpha = 0.45$, whereas the thick solid line is the ionization rate from nonlocal pseudopotentials with spin-orbit.

the two different band structures is quite large and, as a consequence, the ionization rates critically depend on the band structure used for the calculation. This difference, however, cannot be explained by the energy splitting of the split-off band alone, as we have explored for *indirect* gap materials.

The density of states from local pseudopotentials without spin-orbit is again scaled so that the scaled density of states coincides with what was obtained using nonlocal pseudopotentials and spin-orbit in low energy regions (see Fig. 4). We find that $\alpha = 0.45$ for InAs. Also, the density of states is approximated by Eq. (3) with $s = 1.5$, as shown by a thick dashed line in Fig. 4. Employing Eq. (4), the *scaled* ionization rate for InAs is calculated and plotted as a thick dotted line in the same figure. The *scaled* ionization rate now differs significantly from that of nonlocal pseudopotentials with spin-orbit in *low* energy regions. This deviation demonstrates that the density of states is not the only ingredient required to reproduce the correct ionization rate for direct gap materials. Rather, also the matrix elements play a crucial role in controlling the ionization rate, as in the case of electron-initiated impact ionization.[1]

4. Conclusions

The significance of the energy splitting in the split-off valence band for the calculations of hole-initiated impact ionization rate has been investigated. To attain this objective, we have computed the *ab-initio* ionization transition rates in Ge, Si, GaAs, InAs, and $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ by

employing nonlocal and local pseudopotentials with and without spin-orbit interaction, respectively.

The inclusion of the spin-orbit splitting Δ in the valence band is indeed essential to accurately compute the rate for hole-initiated impact ionization. This fact stresses that impact ionization transitions are *low-energy* processes in the sense that the density of states for the secondary carriers in low energy regions determines the energy dependence of the ionization rates. This is especially true for *indirect* gap semiconductors. For *direct* gap semiconductors, however, the situation is more complicated since the matrix elements also play a key role in determining the ionization rates.

Acknowledgments

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