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AUGER RECOMBINATION IN LOW-DIMENSIONAL STRUCTURES

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Abstract—The results of calculations of Auger recombination rates in quantum wells, quantum well wires and quantum well spheres are described and reviewed. The important physical factors influencing the Auger processes are identified and methods of reducing the recombination rate are considered. It is concluded that the rate of Auger recombination is relatively insensitive to dimensionality but that there is the prospect of reducing the rate by modifying the band structure by the use of strain or by exploiting the anisotropy in the electronic structure.

Keywords: Auger recombination, semiconductor lasers, quantum wells, quantum well wires.

INTRODUCTION

Low-dimensional semiconductor structures are of interest for a range of electronic device applications and also provide a rich variety of physical effects that are of fundamental interest [1]. In optoelectronics the quantum well laser has attracted much attention from physicists, device engineers and other workers [2]. The principle of this variant of the conventional semiconductor laser is that the quasi-two-dimensional active region should be able to provide larger gain, low threshold current and less temperature sensitivity. These qualities are essentially the result of the non-zero density of electronic states at the edges of the conduction and valence bands. It is expected that the quasi-one-dimensional quantum well wire could form the basis of a laser with an even higher specification [3] because of the divergence in the density of states at the band edges in this structure. The next step down in dimensionality is to an array of quantum well boxes where the energy levels of bound states are discrete and the boxes play the role of giant atoms [3].

The inspiration for these current and possible future developments comes from a consideration of the optoelectronic and optical properties of the structures embracing concepts such as gain spectrum and optical confinement. However, it is sensible to be vigilant of other processes whose significance may vary with dimensionality and may detract from the benefits mentioned above. One such process is Auger recombination which is well known as a contribution to the temperature sensitivity of conventional semiconductor lasers but has not been extensively studied in low-dimensional structures; experimental measurements of recombination rates are particularly scarce.

This paper reviews some aspects of Auger recombination in low-dimensional structures. Although much of the research discussed has been motivated by a desire to explain and predict the behaviour of lasers, the results have a significance beyond that device. For example, Auger recombination is relevant to the behaviour of other electronic devices such as long-wavelength optical detectors based on narrow gap semiconductors. However, quite apart from device considerations, Auger recombination is an interesting physical process in its own right and the work is of general interest in the study of low-dimensional systems.

Most of the results discussed here are based on the simplest models of low-dimensional structures. For example, simple parabolic sub-bands are assumed and these are taken to be occupied by carriers described by quasi-Fermi levels within Boltzmann statistics. As such, many of the results are intended to show trends or comparisons and to identify important physical factors rather than to provide a quantitatively accurate description.

BASIC THEORY FOR BULK SEMICONDUCTORS

A CHCC Auger recombination process in a bulk semiconductor is shown in Fig. 1. It can be viewed as an electron–electron scattering event in which two electrons in conduction (C) band states 1 and 2 make transitions to final states 1′ in the heavy hole (H) band and 2′ in the conduction band. Fermi's Golden Rule gives the rate of recombination per unit volume R as [4]

$$R = \frac{1}{V}\frac{2\pi}{\hbar}\sum_{\substack{\text{all}\\\text{states}}} P|M|^2\,\delta(E_1 + E_2 - E_{1'} - E_{2'}), \quad (1)$$

where V is the volume of the system, E_i are the energies of the states involved and P is the statistical

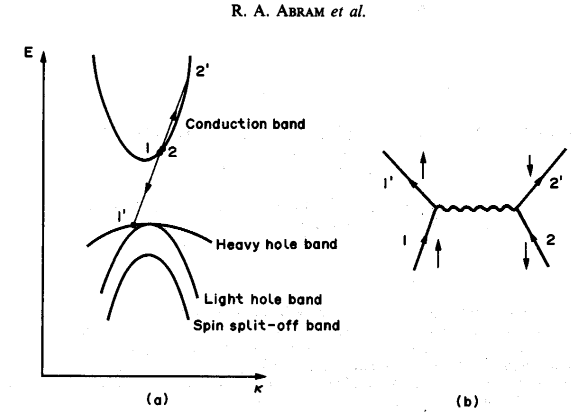

Fig. 1. (a) A CHCC Auger process in a direct gap semiconductor. (b) Diagrammatic representation of the electron–electron collision in a CHCC Auger process (other arrangements of initial and final spins are also possible).

factor that takes account of the occupancies of the states required for the transitions. M is the transition matrix element and for the particular spin configuration shown in Fig. 1 it has the form

$$M = \int \psi_{1'}^{*}(\mathbf{r}_1)\psi_{2'}^{*}(\mathbf{r}_2)\frac{e^2}{4\pi\epsilon\epsilon_0|\mathbf{r}_1 - \mathbf{r}_2|} \times \psi_1(\mathbf{r}_1)\psi_2(\mathbf{r}_2)\mathrm{d}^3\mathbf{r}_1\mathrm{d}^3\mathbf{r}_2, \quad (2)$$

where ϵ is the relative permittivity of the intrinsic semiconductor and $\psi_m(\mathbf{r})$ are the electron wavefunctions. The screening of the electron–electron interaction by free carriers has been omitted because this is normally negligible for the dynamic screening appropriate to Auger recombination [5].

When the wavefunctions are written in the Bloch form and $|M|^2$ is evaluated using (2) it is found that

$$|M|^2 \propto \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_{1'} - \mathbf{k}_{2'}). \quad (3)$$

The delta function provides a wavevector conservation condition in (1) which already contains explicitly the requirement of energy conservation. The demands of energy and wavevector conservation mean that the CHCC process is not possible with the initial and final states at the conduction and valence band edges. It turns out that there is a configuration of states that provides the dominant contribution to the sum in (1) [6]. This "most probable process" has $\mathbf{k}_1 = \mathbf{k}_2$ and non-zero, and $\mathbf{k}_{1'} = -\mu^{-1}\mathbf{k}_1$, where μ is the ratio of the conduction band electron mass to the heavy hole mass. The total energy required to excite the two electrons and the hole from the band edges to these states is $\mu E_g(1+\mu)$, where E_g is the band gap energy, and this is manifested in an activation energy for Auger recombination. When the electron and hole concentrations, n and p respectively, are excited to levels far in excess of their equilibrium values, but remain non-degenerate, the Auger recombination rate can be written as

$$R = Cn^2p. \quad (4)$$

The dependence on n and p arises from the requirement of two electrons and one hole for each process. The Auger coefficient, C, is independent of carrier concentration but is proportional to exp $(-E_a/kT)$, where the activation energy, $E_a = \mu E_g/(1+\mu)$, originates as described above.

QUANTUM WELL

To begin the discussion of Auger recombination in a quantum well we consider the CHCC recombination of an electron and a hole, both of which are in their respective ground sub-bands, and the excitation of another electron within the lowest conduction band sub-band as shown in Fig. 2(a). The discussion follows closely the work of Smith *et al.* [7]. The excited electron will normally have an energy which is far in excess of the top of the conduction band well but it can still be bound to the well. This is because most of its kinetic energy is due to its motion parallel to the well layer and the remaining kinetic energy perpendicular to the layer is not sufficient for it to escape. For simple parabolic subbands the Auger rate is found to be

$$R \propto n^3 \exp\left(\frac{-\mu}{1+\mu}\frac{\Delta E}{k_BT}\right), \quad (5)$$

when the ground sub-bands are excited with equal, large concentrations n of electrons and holes. Equation (5) is similar to the result (4) for the bulk material except that ΔE is the energy gap of the quantum well, i.e. the energy separation of the ground electron and hole sub-bands.

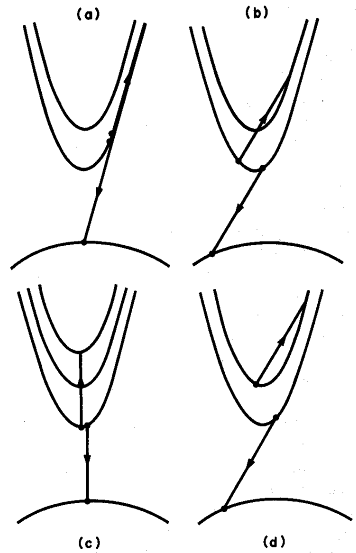

Fig. 2. Electron transitions for some CHCC Auger processes in the quantum well system.

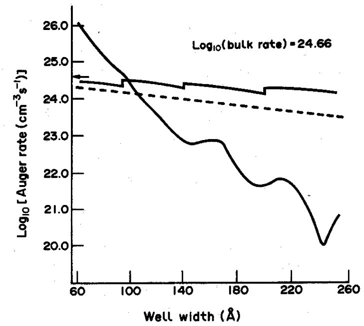

Fig. 3. Auger recombination rates in a QW. The full "sawtooth" curve is the total bound–bound Auger recombination rate in a 1.3 μm InGaAs–InP QW. The temperature has been taken to be 300 K, and the injected carrier density is 10^{18} cm^{-3}. The broken curve is the bound–bound rate for carriers in ground state sub-bands only. The oscillatory full curve is the bound–unbound Auger rate (with bound states being in the ground state sub-bands). The arrow indicates the Auger recombination rate in bulk 1.3 μm InGaAsP for the same temperature and injected carrier density. Realistic overlap integrals [15, 16, 18] have been used.

Figure 2(b) shows another process in which the excited electron transfers to another sub-band. The matrix element M will of course differ from that of the intrasub-band transition case and if the sub-bands are numbered $n = 1, 2, 3, \ldots$ in energy order then transitions for which Δn is odd give $M = 0$, a result that can be deduced by symmetry considerations. Another influence on the rate is the activation energy whose origin was described in the previous section. When a change of sub-band occurs for the excited electron the activation energy is reduced. To see this, consider Fig. 2(c) where the difference in sub-band energies and the effective band gap are equal. Transitions involving band edge states are now possible and will also be favoured by the carrier statistics. Because the carriers are not excited away from the band edge for the dominant process, the activation energy is zero for this case and this acts to enhance the Auger rate although the matrix element M is also an important influence. In fact, for the common semiconductor systems, this process is only possible when the upper conduction sub-band corresponds to an unbound state of the well as discussed later.

There are also processes in which the excited electron undergoes an intrasub-band transition in a higher sub-band, as shown in Fig. 2(d). Here M normally has a magnitude similar to that for Fig. 2(a) but the process is less likely because there are fewer electrons in these higher sub-bands. In addition to the transitions already considered, there are further processes which involve different sub-bands for the recombining carriers.

So far the discussion has concentrated on transitions between bound states of the quantum well but, as pointed out earlier, the structure also has unbound states and transitions involving these should be considered. These unbound states can be viewed as a continuum of sub-bands rather than a discrete set as for the bound states. With this picture the calculation can be carried out in a similar way to that for the bound states except that the summation over sub-bands becomes an integral. It turns out that these transitions can make a significant contribution to the Auger rate, particularly at small well widths. Unbound–unbound transitions are not significant because of the small concentration of carriers assumed for these states.

Figure 3 shows the results of an Auger rate calculation for a 1.3 μm InGaAsP–InP quantum well laser with electron and hole concentrations of 10^{18} cm^{-3} at 300 K. The rate is given as a function of well width, the composition being varied to keep the effective band gap at the value appropriate to 1.3 μm optical emission. The bound state contribution includes all the significant processes described above. The sawtooth structure of this curve comes from the new states that are bound by the well as it is widened. The principal effect of the extra sub-bands at intermediate well widths is to act as receivers for the excited electrons; they are not sufficiently populated to play any other role.

The total bound state rate can be compared with the contribution from the process shown in Fig. 2(a) (where the excited electron remains in the first sub-band) and given as a dotted curve in Fig. 3. At small and intermediate well widths the bound–unbound contribution is dominated by electrons initially in the first sub-band. The structure in this contribution comes largely from the matrix element M for these processes. In particular, the minima are due to M vanishing for the transition with zero activation energy [as in Fig. 2(c)] which is normally the dominant contribution. $M = 0$ can occur as a result of the rapidly oscillatory wavefunction of the state $2'$. At small well widths the bound–unbound processes can become dominant. The sharp decrease for large well widths is due primarily to the high spatial frequency of the final state wavefunction of the excited electron which reduces the matrix element.

It is clear from Fig. 3 that the ground state sub-band rate gives a fairly good guide to the total Auger rate in the well width range 100–200 Å. Taylor *et al.* [8] have presented formulae giving the ratio of the ground state process rate to that in the bulk assuming equal carrier concentrations in both cases. For the CHCC process this is

$$\frac{R_{QW}}{R_B} = \frac{9\sqrt{\pi}}{8}\left(\frac{2\mu+1}{\mu+1}\right)\left(\frac{k_B T}{E_a}\right)^{1/2}, \tag{6}$$

where $E_a = \mu \Delta E/(1+\mu)$ is the activation energy. Results are also given in that paper for other Auger processes such as CHSH and CHLH.

For materials of relevance to long-wavelength semiconductor lasers it is usual for $E_a \sim k_B T$ and then it follows from (6) that the Auger rates in the quantum well and the bulk are roughly the same. In semiconductor lasers it is desirable to reduce Auger recombination and although the act of confinement of the carriers in a quantum well does have a beneficial effect on the gain spectrum it is apparent that it does not have a major effect on the Auger recombination. Of course, a reduction in Auger recombination is possible as a result of a decrease in the threshold carrier concentration due to any improvement in the optical properties, but the exponential dependence of the Auger rate on ΔE has worrying implications in view of the trend towards longer-wavelength lasers for optical communications and other applications. These general conclusions seem to be borne out by the very limited amount of experimental work [9] and by other recent theoretical studies, notably that of Landsberg and Adams [10].

However, Adams [11] has recently proposed that Auger recombination can be dramatically reduced in strained layer quantum well structures even in the absence of any decrease in carrier density. The proposal is to have a quantum well structure in which the well layer is in biaxial compression. The combination of confinement and strain can produce a ground state hole sub-band which close to $\mathbf{k} = 0$ has a small effective mass (perhaps only 50% greater than the bulk light hole mass). It is possible to achieve a "light hole region" which is sufficiently extensive in $\mathbf{k}$ space and sufficiently well removed in energy from the first excited sub-band that the large majority of holes reside in it. The effect of the small mass for holes can be seen from (5). The value of μ can be increased several-fold and the resulting increase in the activation energy can reduce the Auger rate by orders of magnitude.

There have been a number of studies of the effect on photoluminescence and optical absorption of an electric field applied transverse to a quantum well (see, for example, [12]). The principal effects are (a) a reduction in the energy separation of the ground state sub-bands and an accompanying low-energy tail in the optical spectrum—essentially the analogue of the Franz–Keldysh effect, and (b) a decrease in the rate of recombination due to the reduction in the overlap of the electron and hole wave functions. It is therefore interesting to see how an electric field affects Auger recombination in a quantum well. For definiteness we continue to consider the CHCC process. Just as with radiative recombination, the smaller overlap of the electron and hole wavefunctions acts to reduce Auger recombination. However, the decrease in the quantum well band gap also reduces the activation energy and therefore tends to enhance the rate. To estimate which of these contrary influences is most effective we can consider the simplest possible case—identical parabolic wells in the conduction and valence bands. A graded band gap system would not produce identical wells in both bands but the result is not expected to be very sensitive to the shape of the well or the ratio of band offsets. Consider wells of the form

$$E_c = E_{co} + \tfrac{1}{2}Ax^2$$
$$E_v = E_{vo} - \tfrac{1}{2}Ax^2$$

as shown in Fig. 4(a). When an electric field F is applied, the quantum well band structure becomes that shown in Fig. 4(b). The parabolic wells retain their shape but separate in space and move closer in energy. The energy gap is reduced by $|e|^2F^2/A$ and, because of the accompanying change in the activation energy, the Auger rate is enhanced by a factor

$$\exp\left(\frac{\mu}{1+\mu}\frac{|e|^2F^2}{A}\frac{1}{kT}\right).$$

The separation in space causes the overlap integral of the wavefunctions of the recombining carriers to be reduced by roughly a factor of

$$\exp\left(2\alpha^2\frac{|e|^2F^2}{A^2}\right),$$

where $\alpha = (m_c A/\hbar^2)^{1/4}$ and it is assumed that $\mu \ll 1$. It follows that the rate will increase as a result of an applied field if

$$\frac{\mu}{1+\mu}\frac{\delta E_c}{kT} > 1, \tag{7}$$

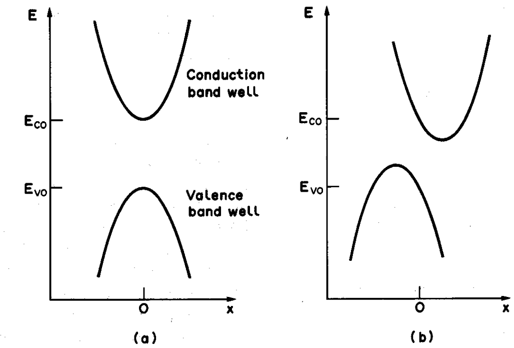

Fig. 4. A QW with identical parabolic wells in the conduction and valence bands (a) without an applied electric field, and (b) with an applied electric field.

where δE_c is the sub-band edge energy separation in the conduction band. This condition is unlikely to be satisfied, except at low temperatures when Auger recombination is small anyway, because μ is typically of the order of 0.1.

QUANTUM WELL WIRE

An ideal quantum well wire laser is expected to have a better gain spectrum than either a quantum well or a conventional double heterostructure laser (see Arakawa *et al.* [3] for a discussion). If such a laser could be fabricated it should have a lower and less temperature-dependent threshold current, provided efficient optical confinement is arranged and there is no significant increase in adverse effects such as non-radiative recombination. With the last condition in mind it is interesting to examine Auger recombination in this system.

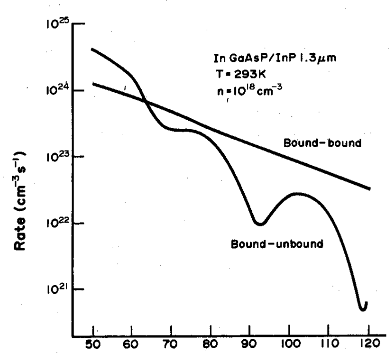

Fig. 5. CHCC Auger rates calculated for a cylindrical quantum well wire using a finite well model with band offsets of $\Delta E_c:\Delta E_v = 2:1$. The overlap integrals used are taken from a pseudopotential calculation, and are appropriate for a wire fabricated with its axis in the ⟨110⟩ direction. Band mixing effects have not been included. (The bound states are all taken to be in ground state sub-bands.)

Taylor *et al.* [13] have reported calculations of CHSH and CHCC processes in an InGaAsP–InP quantum well wire of square cross-section designed to emit light at 1.3 μm. In this work, only transitions involving bound states were considered and the ratio of the Auger recombination rates in quantum well wires to quantum wells was found to be

$$\frac{R_{\mathrm{QWW}}}{R_{\mathrm{QW}}} \cong \left(\frac{k_B T}{E_a}\right)^{1/2}, \tag{8}$$

where E_a is the activation energy for the process and factors of order unity have been neglected to give the approximate relation. Equation (8) demonstrates that the step in dimensionality from two to one has a similar effect to that from three to two.

In view of the importance of bound–unbound processes at small well widths in the quantum well it is of interest to consider these processes in the quantum well wire. The calculations of Taylor *et al.* referred to above were carried out using an infinite square well potential model for a wire of square cross-section. If transitions to unbound states are to be included it is necessary to use a finite potential well and, since the Schrödinger equation for all space is not separable for the potential well of a square wire, it is much more convenient to consider a wire of circular cross-section.

Figure 5 shows the Auger recombination rates for the CHCC ground state sub-band process and for the ground state sub-band-unbound process as a function of wire radius. The general features are similar to the quantum well results and no new effects are in evidence.

The use of strain is a possible way of reducing the Auger rates in the quantum well wire just as in the

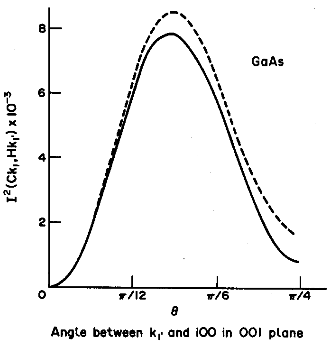

Fig. 6. The modulus-squared of the conduction–heavy hole overlap integral ($|I_{CH}|^2$) as a function of θ, the angle the heavy hole wavevector makes with the x-axis in the xy-plane. The conduction band wavevector is zero, and the heavy hole wavevector is 0.2 $(2\pi/a)$ with a the lattice spacing. The curves are for GaAs; the broken curve is from a pseudopotential calculation, and the full curve is from a 15 band $\mathbf{k}\cdot\mathbf{p}$ calculation.

quantum well. However, Takeshima [14] has made another suggestion, which makes use of the strong anisotropy of the overlap integral between the conduction band and heavy hole band Bloch functions. The matrix element in (3) gives

$$|M|^2 \propto \left|\int u_{1'}^*(\mathbf{r})u_1(\mathbf{r})\,d^3\mathbf{r}\right|^2 \left|\int u_{2'}^*(\mathbf{r})u_2(\mathbf{r})\,d^3\mathbf{r}\right|^2, \quad (9)$$

where 1, 2 and 2′ are conduction band states and 1′ is a heavy hole state. The second integral in (9) is close to unity for all states 2 and 2′ in the Γ minimum of the conduction band, but the first integral has a strong dependence on the wavevectors $\mathbf{k}_1$ and $\mathbf{k}_{1'}$. For the dominant process in bulk material $\mathbf{k}_1$ and $\mathbf{k}_{1'}$ are antiparallel, with $\mathbf{k}_1 \ll \mathbf{k}_1'$. Figure 6 from Brand *et al.* [15], (see also [16]) shows the way in which the squared magnitude of the overlap integral varies with $\mathbf{k}_{1'}$ in the xy-plane when $\mathbf{k}_1 = 0$. The strong directional dependence is clear. Takeshima [14] has pointed out that in the quantum well wire the direction of $\mathbf{k}$ is fixed by the wire axis and, by a suitable choice of wire axis direction, it should be possible to reduce the Auger recombination rate considerably. What is not clear is how much the result will be affected by the mixing of bulk bands that results from the quantum well wire confinement. Until recently that question appeared difficult to answer because the overlap integral results were derived from large-scale numerical band structure calculations. However, recent developments in the theory of the band structure of low-dimensional structures (see for example [17]) and the development by Scharoch (personal communication) of simpler methods of calculation of the overlap integrals, including analytical approximations, means that it is now possible to thoroughly investigate Takeshima's proposal.

QUANTUM WELL SPHERE

It is worthwhile to take the discussion of Auger recombination in low-dimensional structures to its physical limit and to consider processes in quasi-zero-dimensional structures. Here we report some results for the quantum well sphere. The sphere might not be the most feasible shape to fabricate but the calculations are easier for the sphere and the results are not expected to be particularly sensitive to shape.

The bound states of the sphere are discrete because there is no direction in which free motion exists. This has the interesting consequence that bound–bound Auger processes to not generally occur. This is because the band gap transition energy will not have the precise value of any of the discrete state energy separations. In fact, in typical laser materials systems such as InGaAsP–InP the band gap will exceed all the discrete state energy separations. Hence Auger recombination can only occur as a result of bound–unbound processes.

Figure 7 shows the CHCC recombination rate for a range of radii of an InGaAsP–InP system designed to emit at 1.3 μm. The calculations were performed for a single sphere assuming that it is occupied by two electrons and two holes in their respective ground states. With this occupancy condition there is no activation energy for the bound—unbound transition and the rate of recombination is independent of temperature. The calculations do not include excitonic effects, which are likely to be important because of the enforced close proximity of the electrons and holes. The striking feature of the curve in Fig. 7 is that the rate actually falls to zero for certain values of radius. The explanation for the oscillations is the same as that for the other systems discussed, but because of the three discrete states involved there is only one permissible final state energy for the excited electron and the zeros of the matrix element are not obscured by contributions from other transitions. Of course, it should be realized that other Auger processes, such as CHSH, will have vanishing rates at different values of the radius and this phenomenon does not provide a method of eliminating Auger recombination although it may aid its reduction.

Any practical device such as a laser would probably consist of a dense array of spheres. For such an array, it is necessary to consider the statistical distribution of carriers among the spheres to determine the relative probabilities of the various recombination processes. For instance, the CHCC process described above requires at least two electrons and one hole within one sphere although inter-sphere processes are also possible. For example, it is possible for recombination to take place in one sphere and ex-

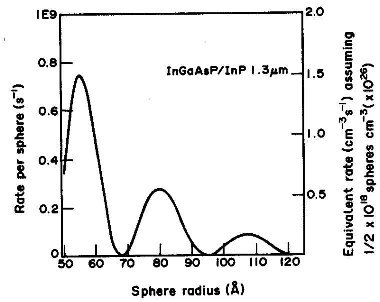

Fig. 7. The bound–unbound CHCC Auger rate calculated for a quantum well sphere. The left-hand scale shows the rate for an isolated sphere, initially occupied by two electrons and two holes. The right-hand scale indicates the equivalent rate for an array of such spheres, in which the injected carrier density is 10^{18} cm^{-3}. These values pertain to an optimum distribution of carriers and provide merely a crude comparison with rates previously discussed.

citation to occur in a neighbouring sphere and this can be described by a simple extension of the theory for a single centre. The statistics of the carrier occupancy of the spheres is a problem akin to that of multiply occupied defect centres as discussed by Landsberg [18], Shockley and Last [19] and others.

CONCLUSIONS

The results presented in the previous sections suggest that confinement by itself does not have a strong effect on Auger rates. That is, Auger recombination is relatively insensitive to dimensionality for given carrier concentrations (per unit volume) n and p. Of course, confinement can still be useful in reducing Auger recombination if it provides a method by which a device can operate just as effectively at lower values of n and p. The confinement of heterostructures can possibly be used more directly to reduce Auger recombination by making use of the effect of strain on the band structure or by taking advantage of anisotropy in the electronic properties of the semiconductor.

These conclusions are based on simple models, which are expected to be reliable for identifying broad trends and important physical factors. However, accurate quantitative calculations require the use of realistic band structures and overlap integrals, Fermi–Dirac statistics and numerical integrals in **k** space over initial and final states.

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