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COMMENT

Comment on 'Monte Carlo simulations of the recombination dynamics in porous silicon'

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Abstract. The results of Monte Carlo simulations of the recombination dynamics in porous silicon have been used to rule out explanations for porous silicon luminescence based on analogies with a-Si:H. In this comment we present arguments showing that the luminescence process of a-Si:H at low temperatures cannot be correctly described by the model system used in the calculations and the results obtained cannot rule out analogies between porous silicon and a-Si:H.

In a recent paper, Roman and Pavesi [1] have reported on Monte Carlo simulations of the recombination dynamics in porous silicon. Their model system consisted of an assembly of Si quantum dots. Different behaviours of the luminescence decay were found for 1D, 2D and 3D lattices.

The authors of [1] suggested that their results for uncorrelated electron–hole pair recombination in 1D lattices can describe the luminescence decay in a-Si:H. Furthermore, they attributed the non-exponential luminescence decay observed in porous silicon to the hopping of excitons, a situation which is very different for the former. Thus, they ruled out explanations for porous silicon luminescence based on analogies with a-Si:H.

In the present comment we show that both ideas outlined in the previous paragraph are not quite convincing. On the one hand the luminescence process in a-Si:H at low temperatures is well described by correlated electron–hole pairs when the density of pairs is sufficiently low. The wide distribution of lifetimes is obtained from radiative tunnelling recombination of a distribution of immobile carriers. On the other hand the luminescence decay in porous silicon at and above the peak of the emission spectum is indeed similar to that found in a-Si:H, i.e. a wide distribution of lifetimes with a peak at relatively long times ($\sim$1 ms) strongly suggesting a radiative tunnelling process. That the wide lifetime distributions may be due to a distribution of carrier distances cannot be ruled out by the kind of simulation performed in [1].

The power law dependence $I(t) \sim t^{-\beta}$ for the luminescence intensity of a-Si:H found in [1] does not strictly correspond to the experimental data at low temperatures [2]. The asymptotic behaviour for temperatures near 100 K is well fitted with $\beta = 3/2$ [2–4], a value much higher than the result of the simulation ($\beta = 0.73$ for 100 K and 0.91 for 300 K). Moreover, this behaviour is asymptotic, and for shorter times the decay cannot be fitted by a simple power law. In fact several articles [5–7] have shown that for a-Si:H the lifetime

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distribution presents peaks, the most important one around 1 ms for good-quality material at low temperatures and low excitation rates, where geminate recombination prevails. The most widely accepted model for radiative recombination in a-Si:H assumes wide lifetime distributions due to a distribution of carrier distances, and is valid for any temperature where the luminescence efficiency is high, including at very low temperatures where the probability of hopping is negligibly small. The distribution of carrier distances arises from carrier diffusion in very short ($\sim$1 ps) time scales. The hopping motion considered in [1] is meaningful only for temperatures above $\sim$100 K, where the quantum efficiency decays dramatically with the temperature. Thus, it should be clear that the hopping process between localized states is not the primary cause of the wide distribution of lifetimes observed in a-Si:H.

After more than 5 years of intensive study, the photoluminescence mechanism of porous silicon is still a controversial subject. As pointed out in [1], the models can be classified into three different groups, each providing explanations for different aspects of the luminescence phenomena. A very recent experimental paper [8] claims that only a chemical model involving oxygen can explain their results, in contrast with the conclusions of [1]. It is our opinion that the luminescence decay curves measured in porous silicon [9] are indeed very similar to those of a-Si:H. The model outlined in [9] discusses the dynamic behaviour of carriers in a band of localized states, without any assumption concerning the nature of these states. We still claim that this dynamic behaviour is very similar in porous silicon and a-Si:H at low and intermediate temperatures, being characteristic of tunnelling recombination of carriers at different distances in high-quantum-efficiency systems. Of course the probability of hopping at time scales much shorter than the effective radiative recombination lifetime is not negligible, and this process can only decrease the quantum efficiency (and the effective radiative lifetime) by enhancing the probability of non-radiative recombination. Further evidence for this process, which occurs in a-Si:H at low and medium temperatures, can be obtained from the decrease in efficiency of porous silicon samples with high connectivity between the silicon islands [10].

We would also like to remark that the use of stretched exponentials for the description of the carrier dynamics, although formally appealing, does not bring much insight to clarify the mechanisms involved. Stretched exponentials can be observed in a wide variety of disordered physical systems [11]. The calculation of lifetime distributions as proposed in [5] and used in [9] provides a much more direct way to identify the processes involved.

In conclusion, we have shown that the results from Monte Carlo simulations obtained in [1] cannot rule out descriptions of the carrier dynamics of porous silicon based on analogies with a-Si-H.

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