Defect studies on silicon and silicon-germanium for PV and optoelectronic applications

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- Defect monitoring in EFG-grown silicon ribbons by room temperature PL spectroscopy
- Monitoring of threading dislocations in Si-Ge alloys

Introduction

- New frontiers for solar grade silicon (use of n-type scraps, refined MG-Si): an old proposal of renewed interest associated to the oil crisis
- New frontiers for microcrystalline silicon as a multipurpose material (PV, optoelectronic)
- New frontiers for EG silicon: strained Si and Si-Ge alloys for high speed electronics and quantum well devices [IR sensors, heterojunction bipolar transistors (HTBs), resonant tunnelling diodes (RTDs)] to cover a field typical of III-V compounds and get integration

Need of defect monitoring and of optimized defect engineering procedures: our group is strongly involved in these activities

Defect monitoring in multicrystalline silicon for PV applications: generalities

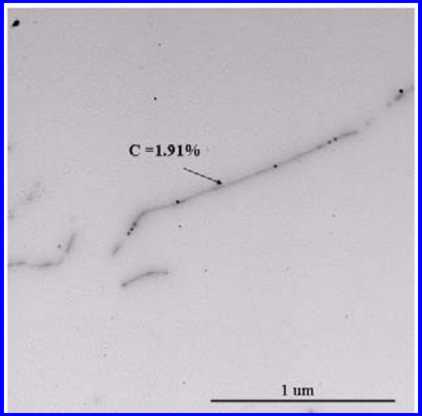
- Extended defects (Dislocations and GBs) in silicon are normally harmful for PV applications, unless dangling bonds are reconstructed or passivated
- Grain size in excess of mm allows effective sun harvesting provided the orientation of GBs is parallel to the carrier drift and diffusion
- Thermodynamics shows that GBs and dislocations are powerful (chemical) traps for impurities: the effect is to increase the minority carrier recombination activity of GBs and dislocatons
- Thermodynamics shows that GBs and dislocations compete with external gettering and passivation sites

Some key examples: Segregation of impurities at GBs and their effect on recombination in DS grown silicon

Effect of non-equilibrium growth & defectivity on the segregation coefficients

Element	K_s (CZ-EG Si)	K_s (DS-MG Si
Cu	6.9 10^{-4}	2 10^{-3}
Cr	1.1 10^{-6}	3.7 10^{-3}
Fe	6.4 10^{-6}	1.6 10^{-4}
Ni	3.2 10^{-5}	9 10^{-4}
Ti	3.6 10^{-6}	2,5 10^{-3}
Zr	1.5 10^{-8}	7.7 10^{-4}

Effect of impurity segregation in n-type mc-Si on recombination activity of GBs



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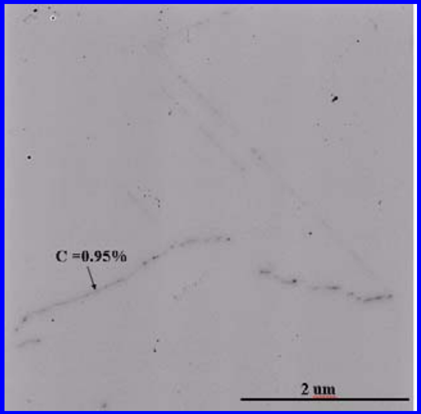

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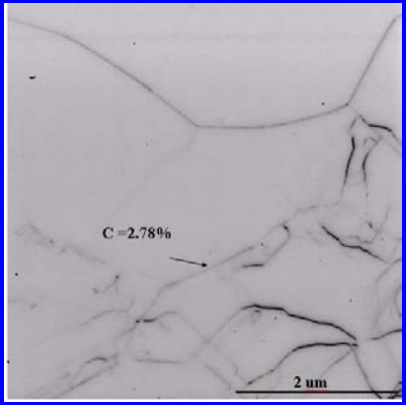

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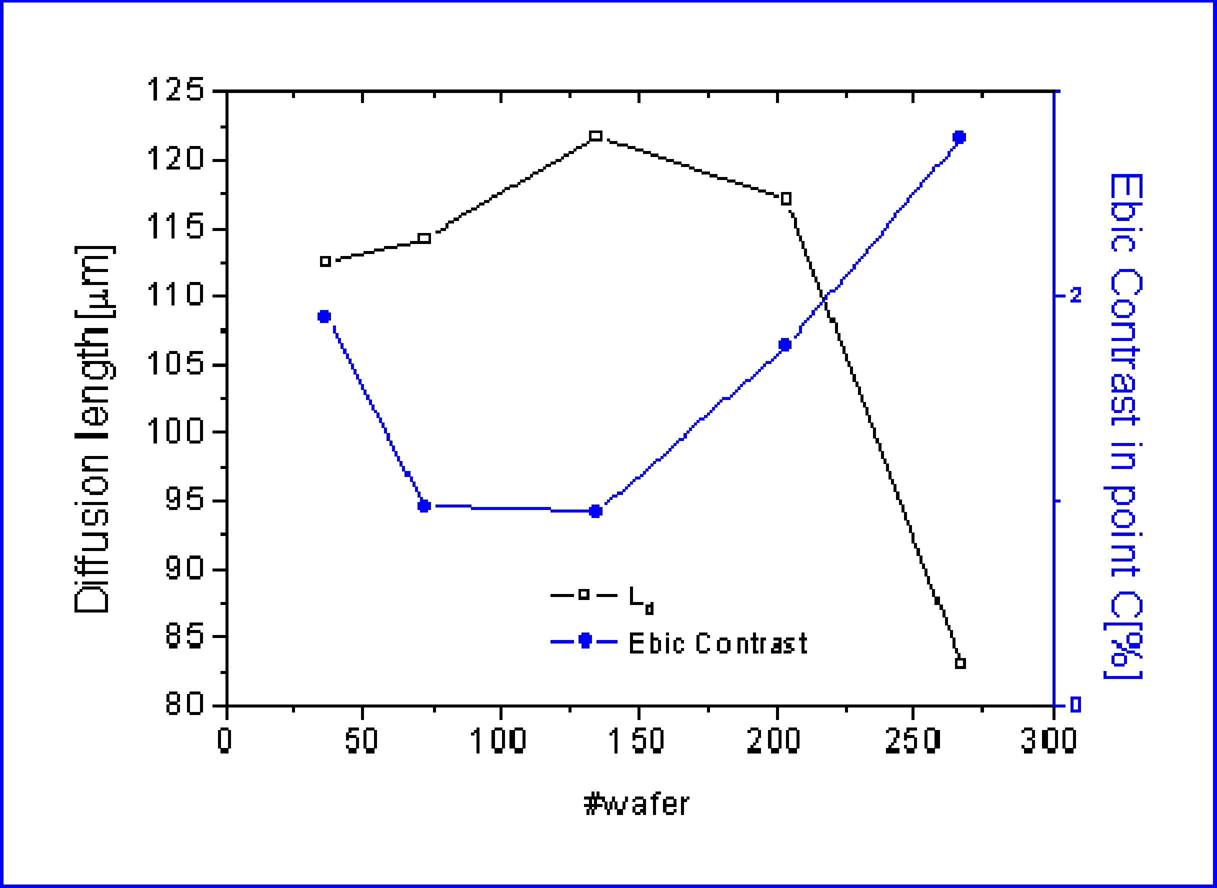
EBIC Contrast vs diffusion length:dependence on impurity segregation in n-type mc-Si



Conclusion

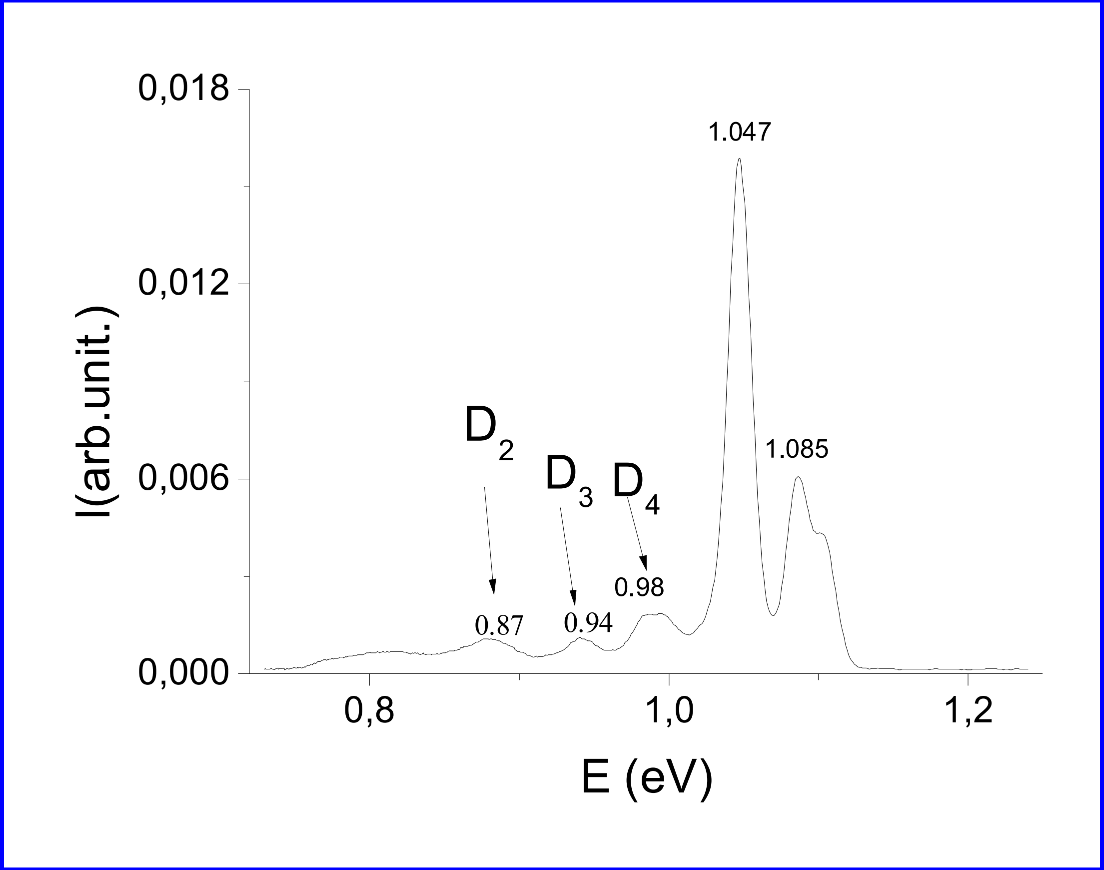
In mc-Si DS-grown from EG feedstocks minute amounts of impurities coming from the crucible, from the feedstock and from furnace misoperation might deteriorate a significant part of the ingot

There is still space for improvements.

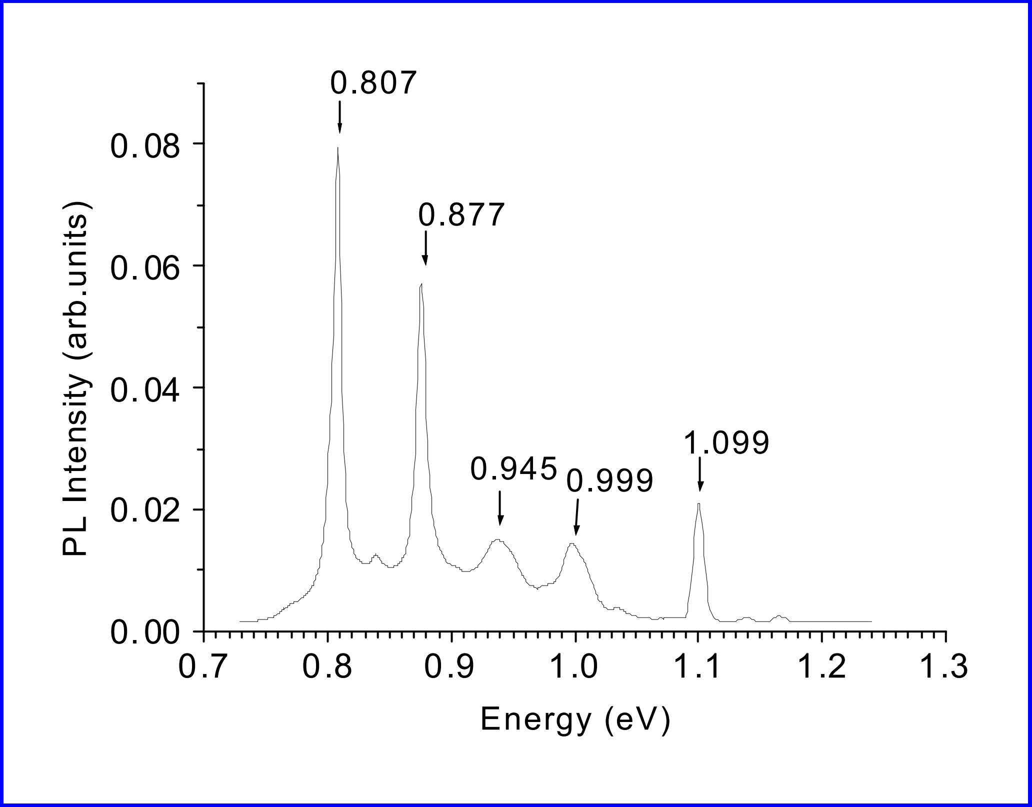
Defect engineering and defect monitoring in n-type DS-grown mc-Si

- Defects identification in mc-Si by PL at 12K
- $POCl_3$ gettering after B-diffusion for junction formation (800-900°C)
- Hydrogen passivation during the AR deposition step (Nitridation)
- Defect monitoring via PL at 12 K and EBIC measurements at room temperature

PL spectrum (12 K) in a GB-rich region

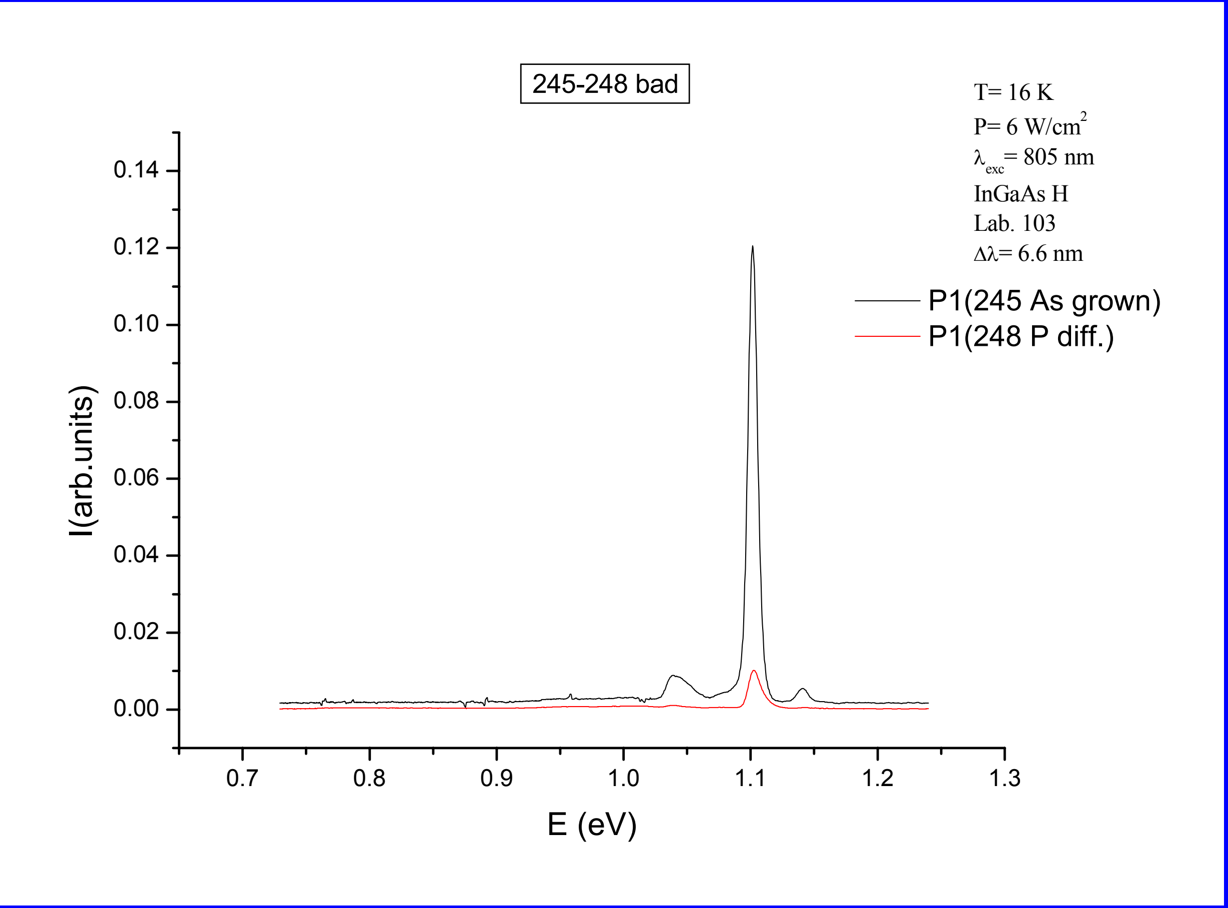


The ≈1.05 eV peak appeares systematically in the presence of GBs, generally associated to dislocation luminescence

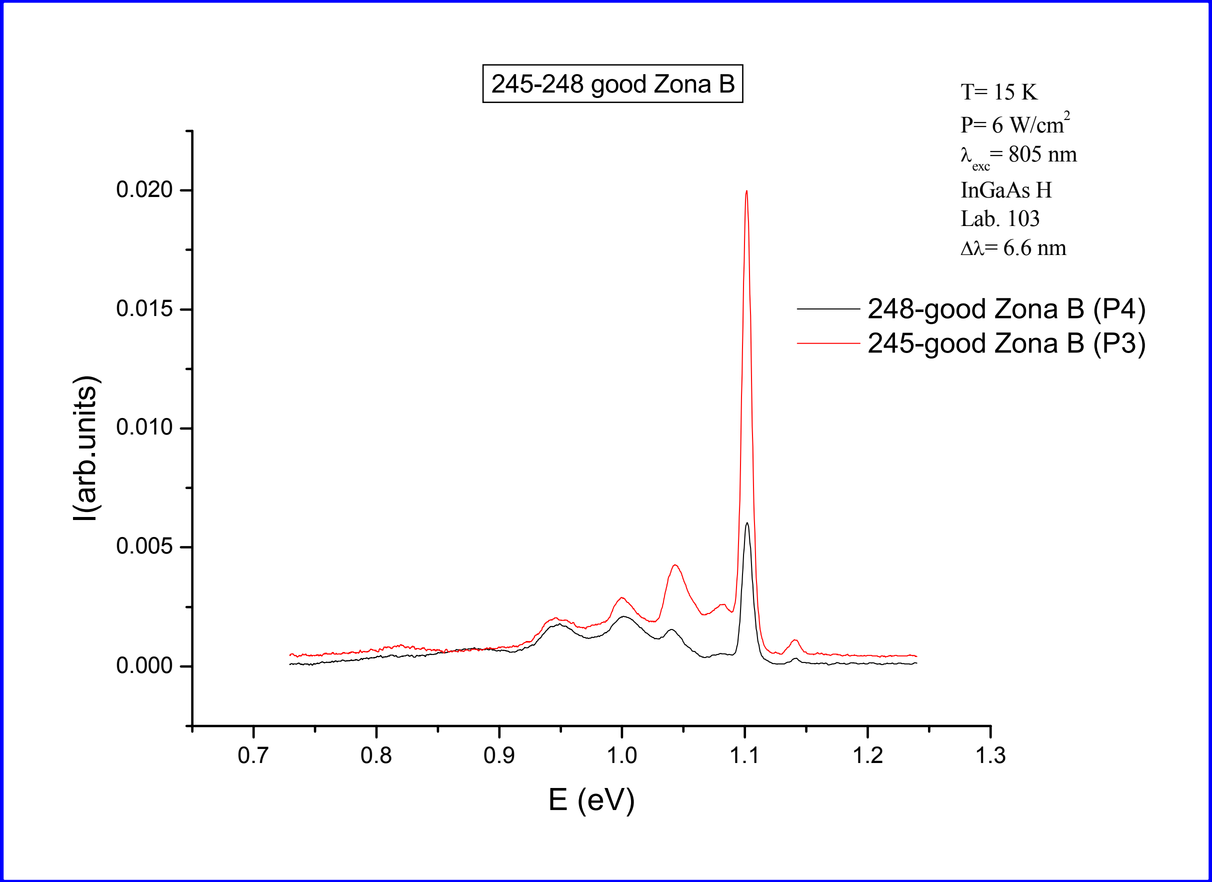


PL spectrum of a dislocated silicon sample

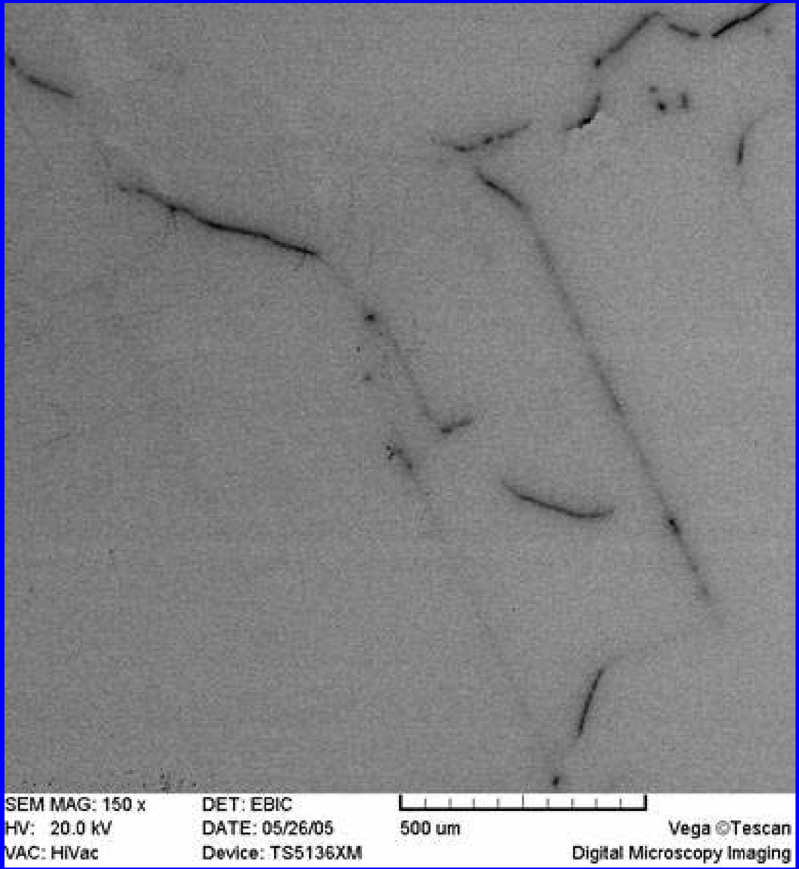
PL spectrum before and after gettering (low lifetime, high defectivity region)



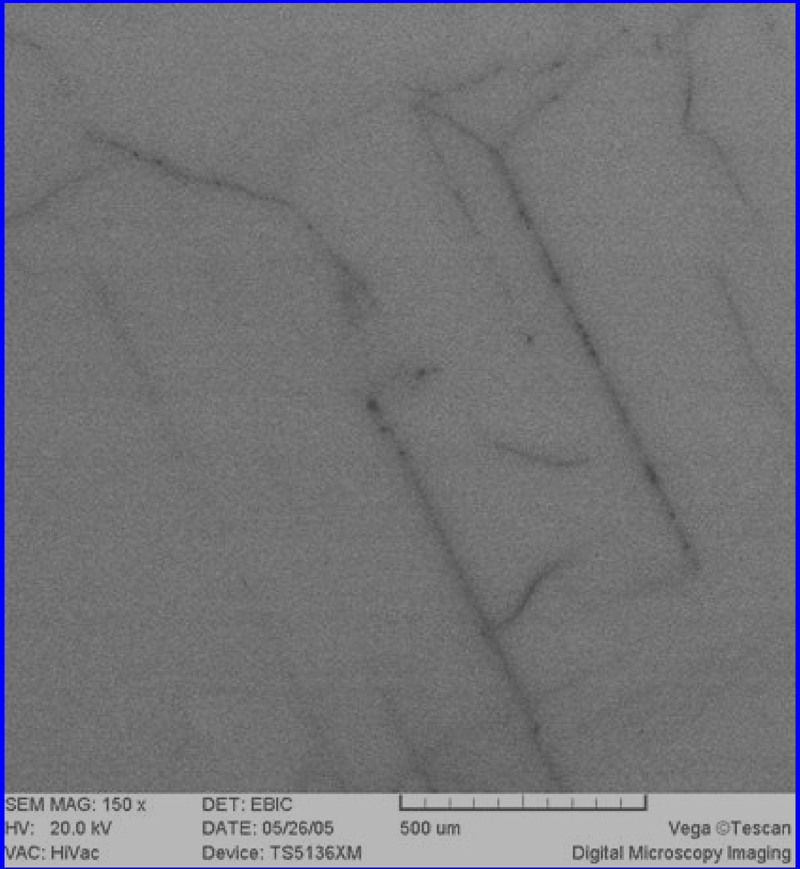
PL spectrum before and after gettering (high lifetime, low defectivity region)



EBIC maps before and after gettering



As grown sample



After POCl3 gettering

Effect of $POCl_3$ gettering

The average lifetime increases from

$\tau_{eff} = 89\ \mu s$ to $\tau_{eff} = 140\ \mu s$

but the (beneficial) effect of gettering on the EBIC contrast is inhomogeneous

Remarks

GBs compete with external gettering in agreement with thermodynamic predictions

$$\mu_{i,GB,dislo} \approx \mu_{i,\,surf}$$

and with literature [T.Buonassisi, M.A Marcus, A.Istratov, M.Heuer, T.F.Ciszek, B.Lai, Z.Cai, E.R.Weber, J.Appl.Phys. 97, 063503 (2005)] who demonstrated, using XR fluorescence, that gettering of iron occurs at GBs. Point-like contrast in the preceeding maps might be due to precipitates

Defect monitoring in EFG-grown silicon ribbons and p-type mc-Si by RT-PL spectroscopy

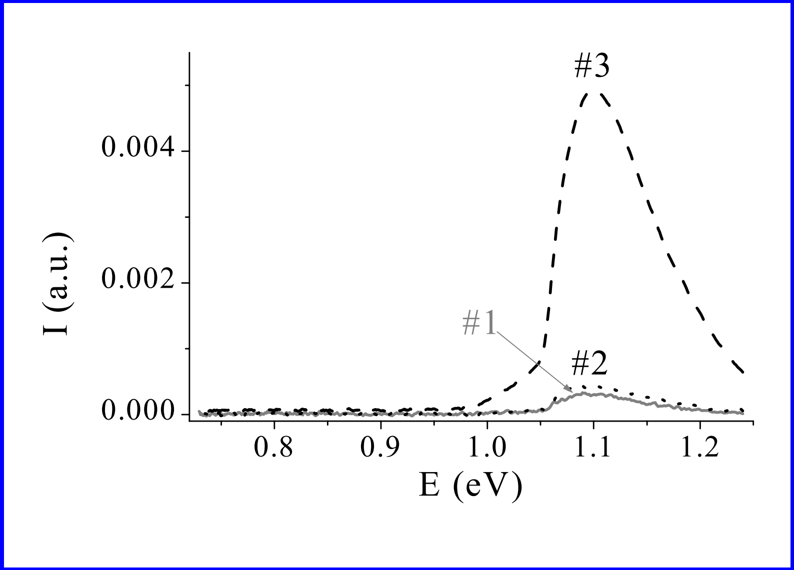
PL measurements at room temperature might monitor material improvements or failures during solar cell processing. Only the excitonic luminescence might be used.

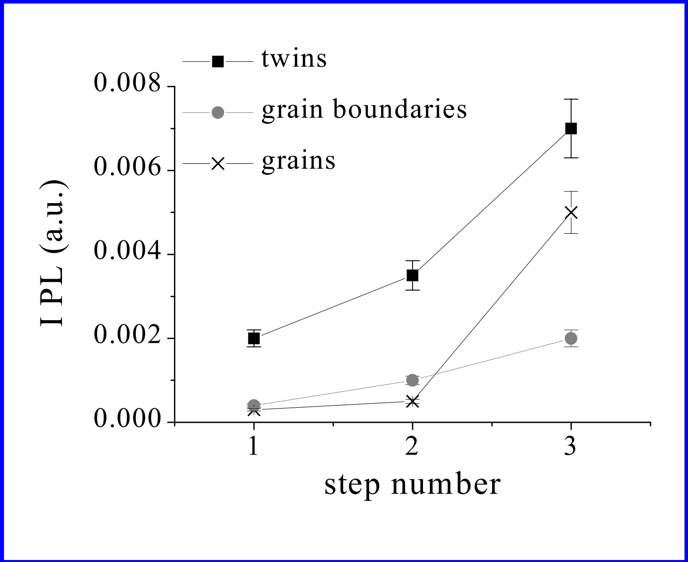
To avoid surface recombination effects, carrier injection is carried out 10 μm deep in the sample

The sample inhomogeneity is accounted for by testing regions with similar morphology

Evolution of the EFG ribbon properties with processing

grain region

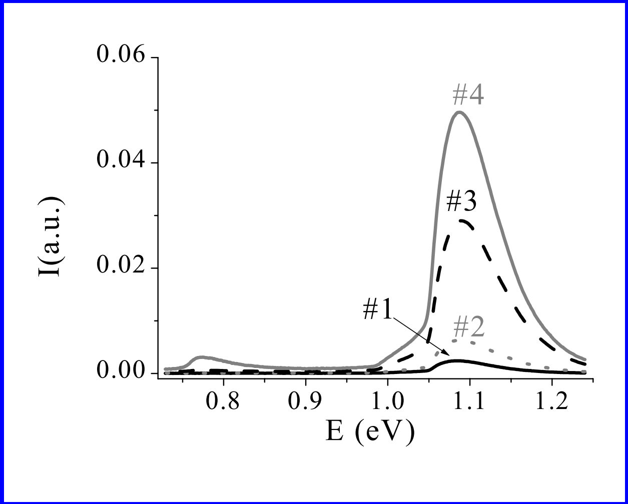


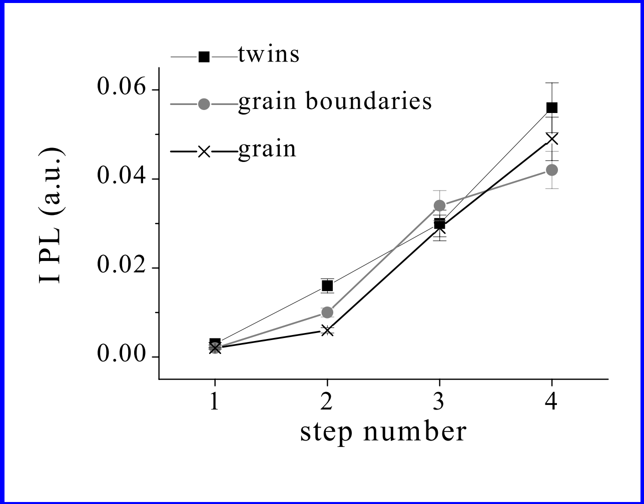


#1 as grown # after junction # after AR coating

Comparison with multicrystalline silicon

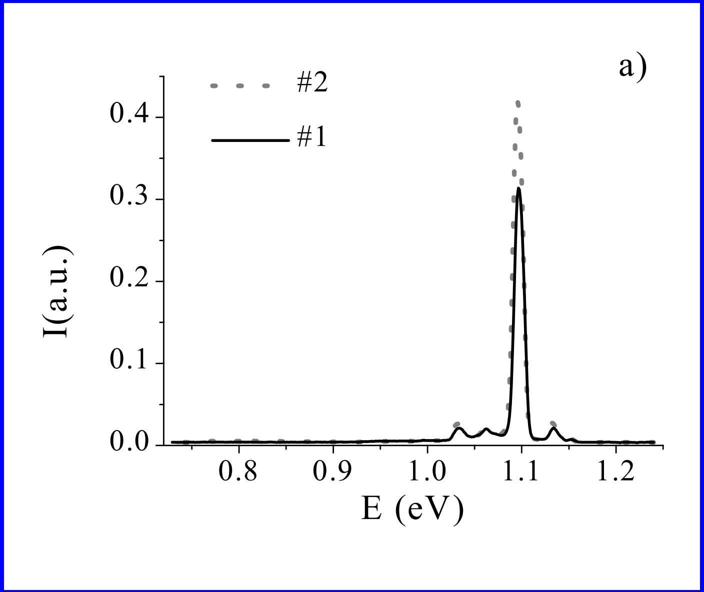
grain region

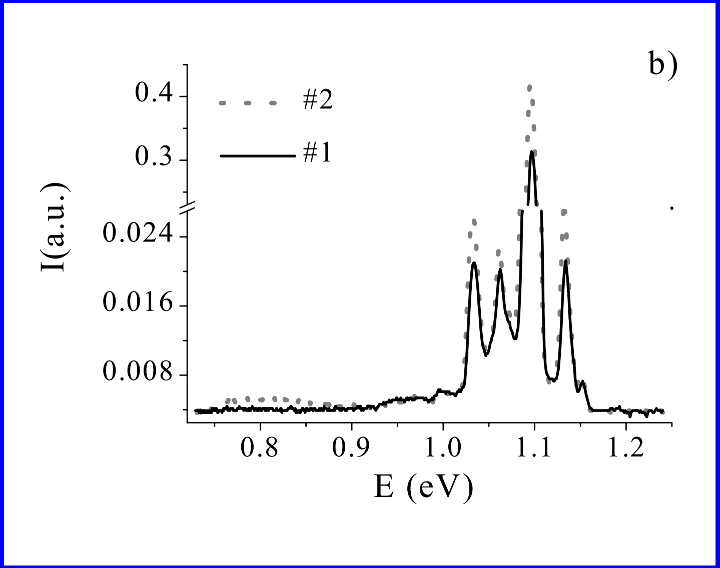




#1 as grown # after junction # after AR coating

Low temperature PL spectra of mc-Si

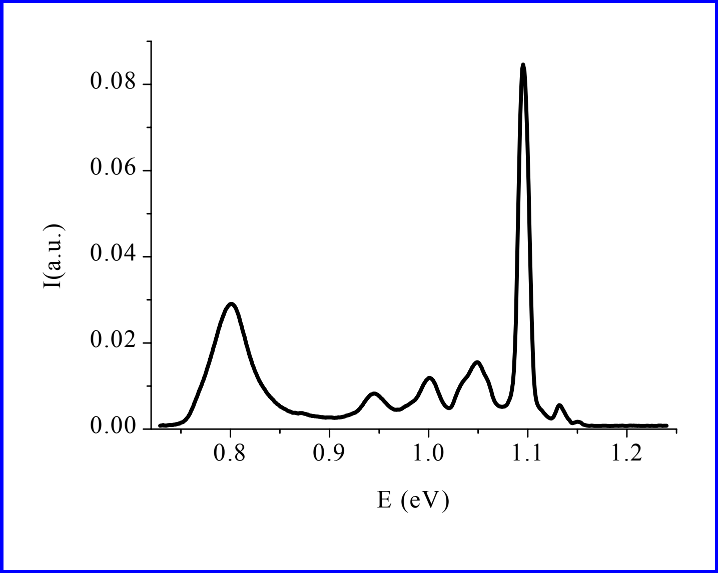


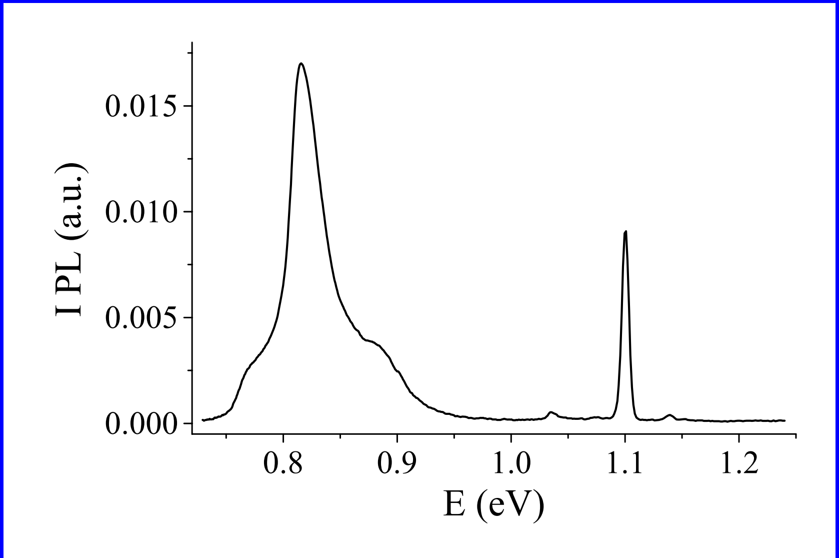


a) PL spectra at 12K of the as grown and texturized mc-Si

b) higher magnification of the same spectrum : the D3+D4 dislocation lines, the phonon replicas and the emission at 1.05 eV are visible)

Effect of P-diffusion/gettering





a)PL spectrum of mc-Si at 12 K after junction formation
b) of dislocated EG silicon after heat treatment at 800°C used to segregate oxygen

Remarks

- RT-PL might be used to follow the effect of process steps on the material performance
- In EFG-Si GBs are not affected by P-gettering and hydrogen passivation, different from mc-Si
- In p-type mc-Si the P-diffusion/gettering induces the segregation of oxygen, the enhancement of the dislocation luminescence

  and the decrease of the excitonic luminescence

Monitoring of threading dislocations in Si-Ge alloys

Problems and advantages of SiGe alloys

- Strained silicon and $Si_{1-x}Ge_x$ deposited on top of silicon substrates allows to extend silicon applications in high speed microelectronics, quantum well devices, remote chemical sensing, thermal imaging, night vision, once limited to III-V semiconductors
- The large lattice mismatch between Ge and Si induces large stresses, which relax via misfit dislocations. By proper graded composition growth dislocations might be confined in a limited region, but some dislocations could cross the epitaxial layer
- Threading dislocations might affect both the concentration of minority carriers (by recombination) and the carrier mobility (by scattering), this last only at high values of N_D

Problems in threading dislocations monitoring

- Selective etches must be tuned vs the Ge concentration [the redox (corrosion) potential of dislocations depends on the Ge concentration]

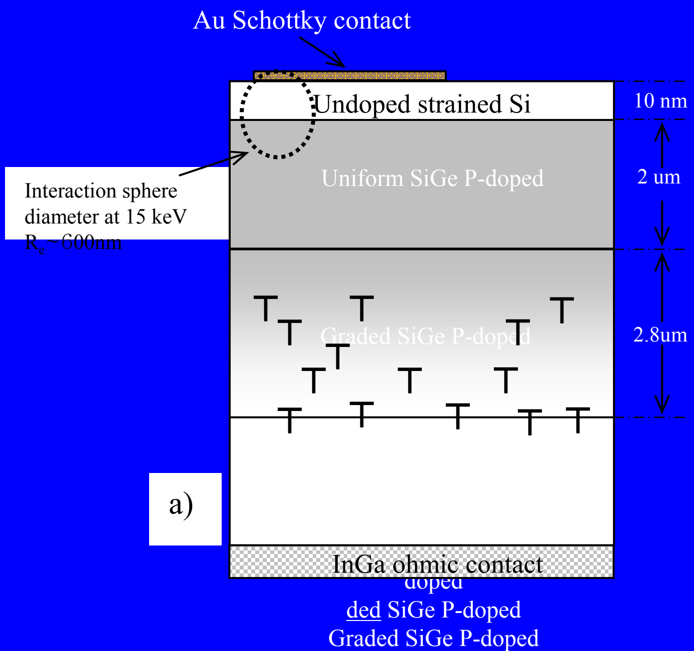
$$\mu_{dislo} = f(c_{Ge})$$

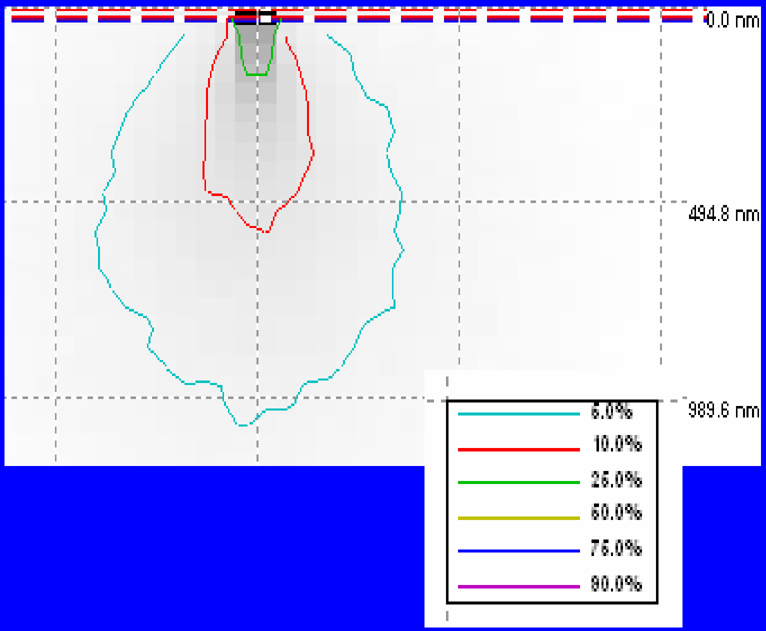
- EBIC might be used to implement the chemical data

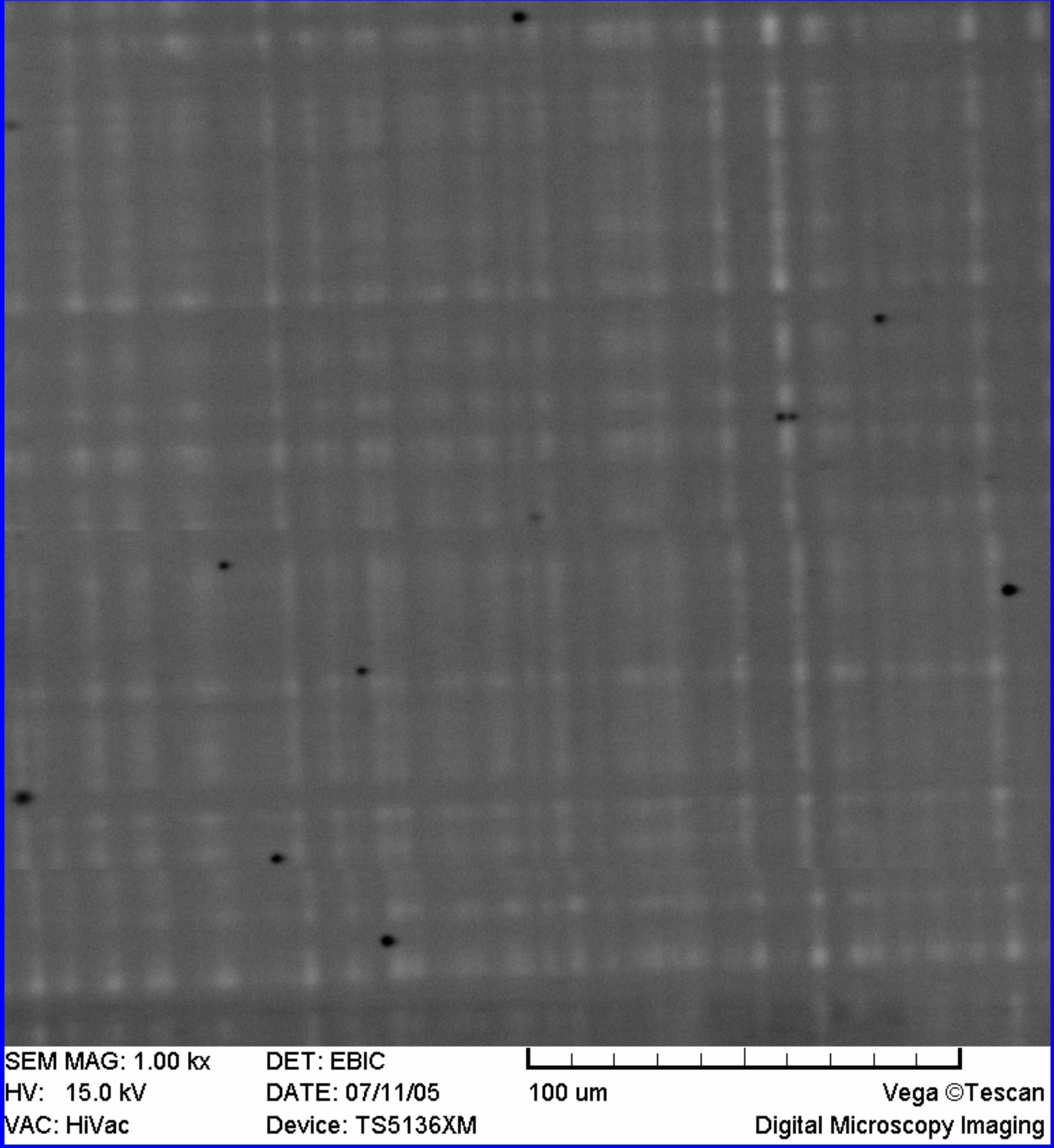
Example

Use EBIC to show the correspondence between the etch pit count and the EBIC count on strained $Si_{0.8}Ge_{0.2}$ prepared using the LEPECVD process

Schematic view of the sample & sample characterization







e.p. c ≈ 1.2 10^4; EBIC count ≈ 2.7 10^4

Conclusion

The combined application of PL, EBIC and diffusion length measurements is of great advantage in applied research activities, addressed at the optimization of solar grade silicon and Si-Ge alloys

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