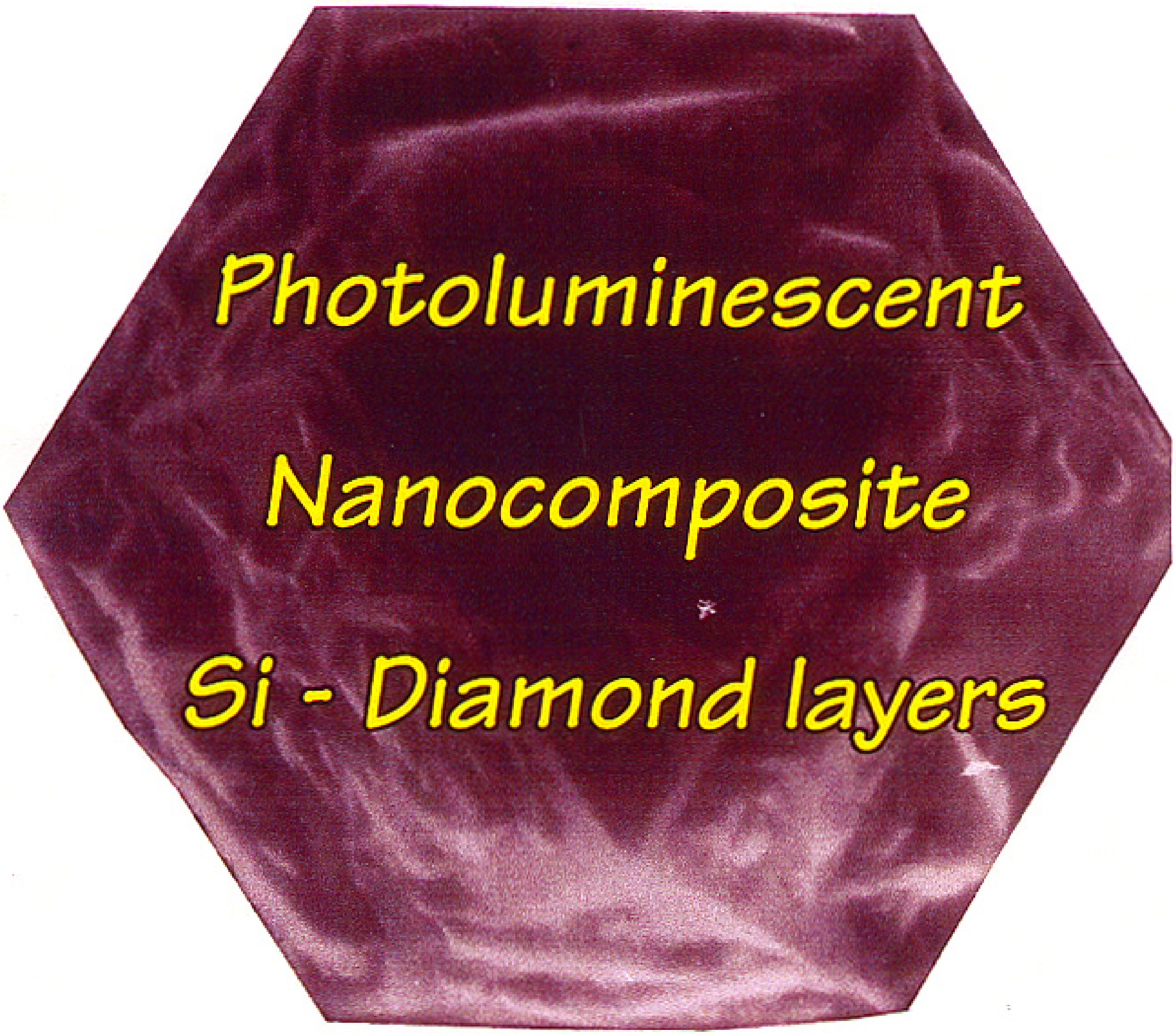

Photoluminescent Nanocomposite Si - Diamond layers

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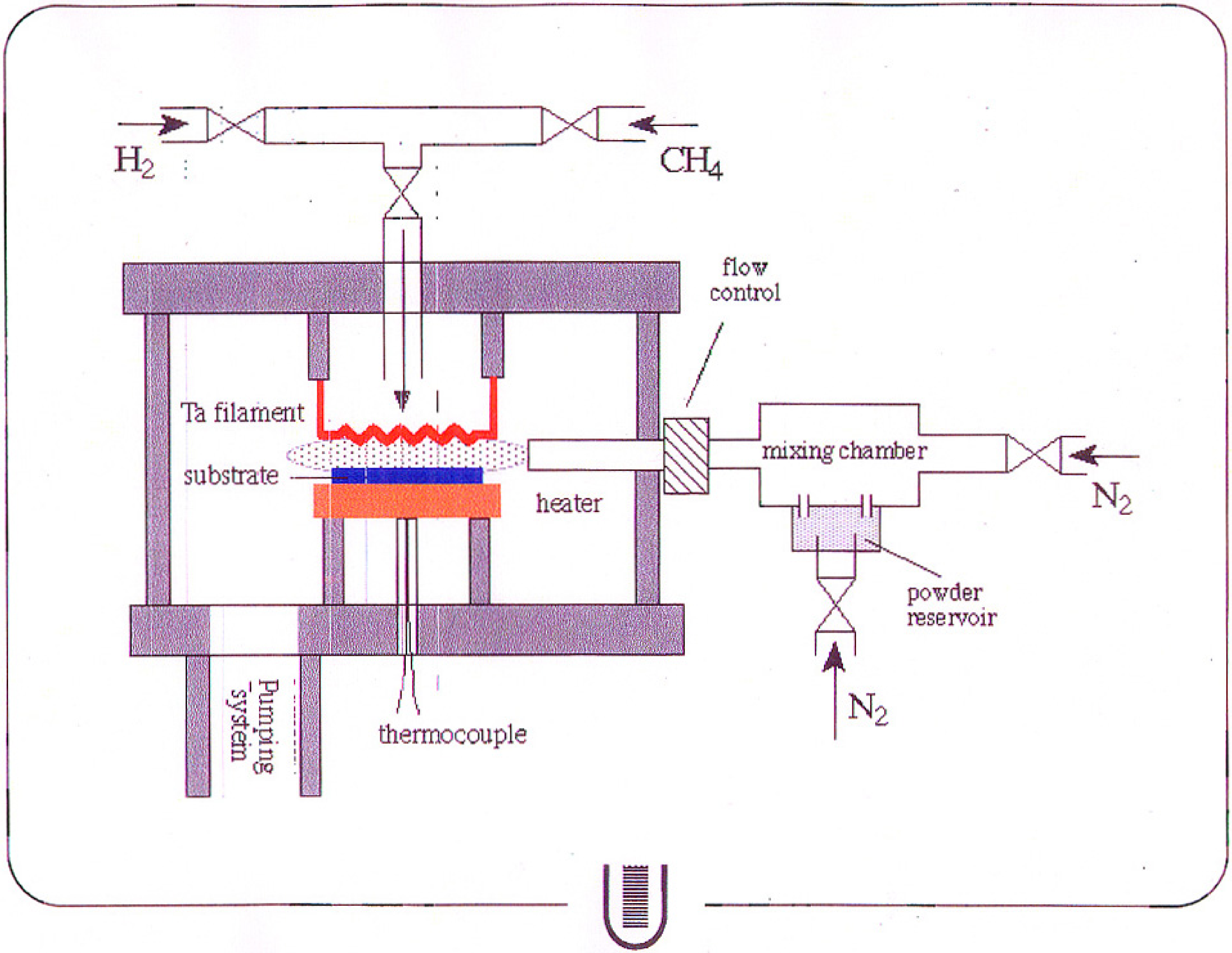
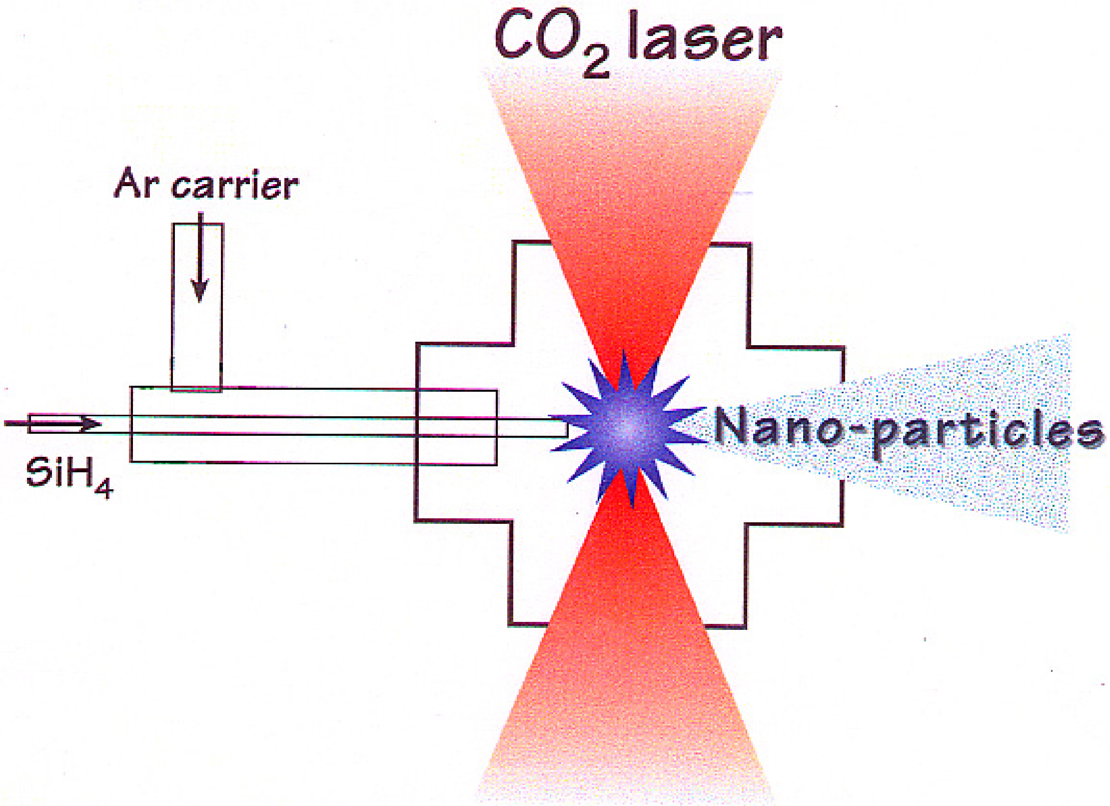


H2
CH4
flow control
Ta filament
substrate
heater
mixing chamber
N2
powder reservoir
N2
Pumping system
thermocouple

Laser pyrolysis

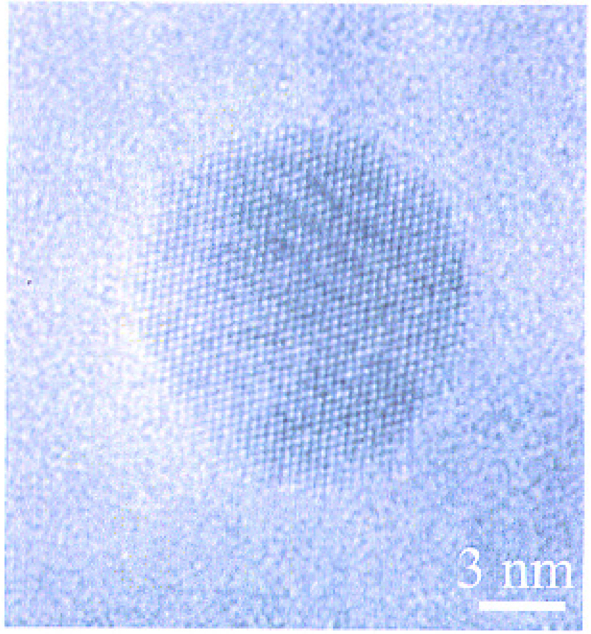


- controlled atmosphere reactor
- small and well defined reaction zone with high temperature gradients
- possibility of probing particles characteristics in the gas phase
- good control with high flexibility of particle size through reaction parameters (2-100 nm)

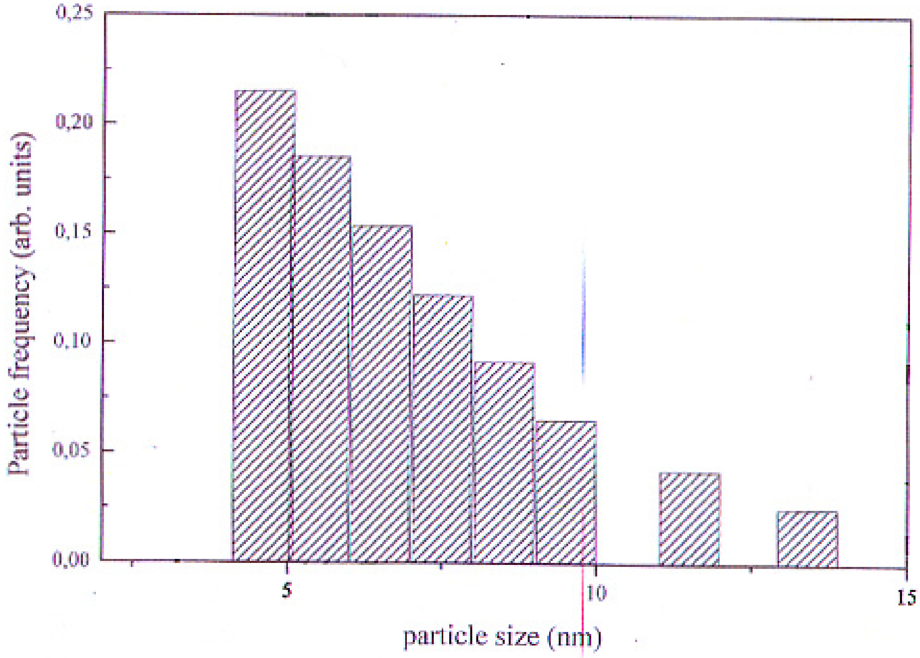
AVERAGE SIZE OF THE USED NANOPARTICLES:

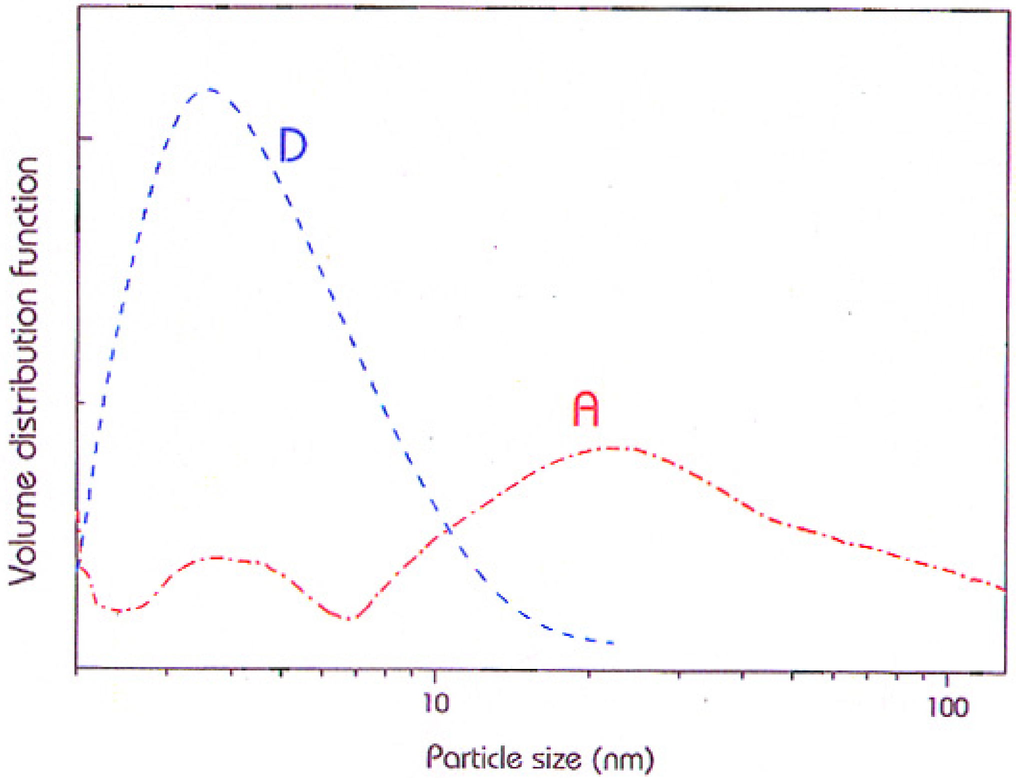
3.6 - 6.2 nm

(2.3÷4.6) (5÷7.3)



Laser-synthesised nano-Si




D
A
Volume distribution function
10
100
Particle size (nm)

DEPOSITION PARAMETERS

FEEDING MIXTURE	1 % CH_4 in H_2
FLOW RATE	200 sccm
GAS CARRIER	Ar
FLOW RATE	30-60 sccm
FILAMENT TEMPERATURE	2180 °C
SUBSTRATE	Si (100)
SUBSTRATE TEMPERATURE	650°C

INSERTED POWDERS
Si nanoparticles

CHARACTERIZATION TECHNIQUES

-Scanning Electron Microscopy

-Atomic Force Microscopy

-Raman Spectroscopy

Ar+ (514.5 nm) at 130 mW

-Reflection High Energy Electron Diffraction

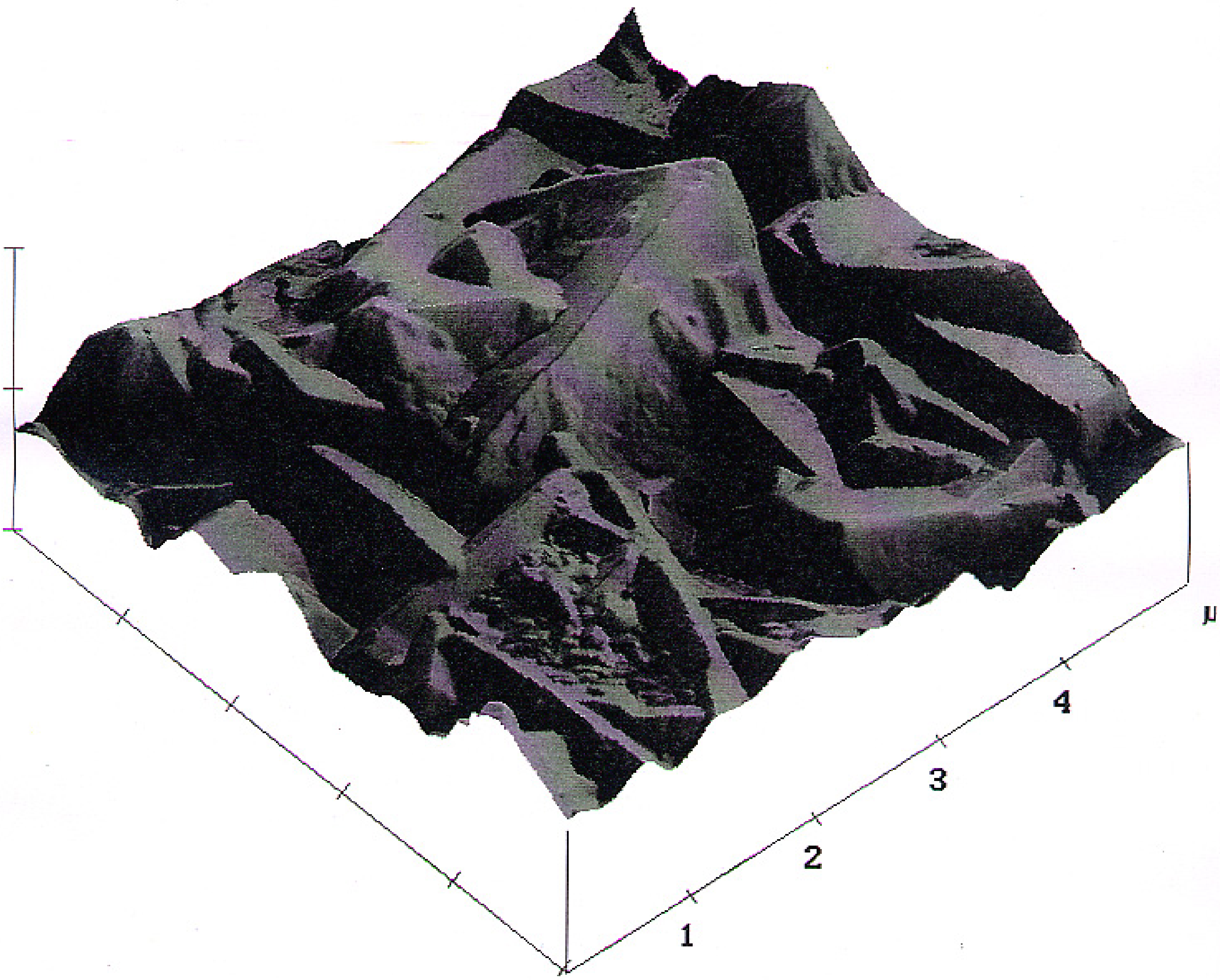
diffraction stage at 60 kV

-Photoluminescence :

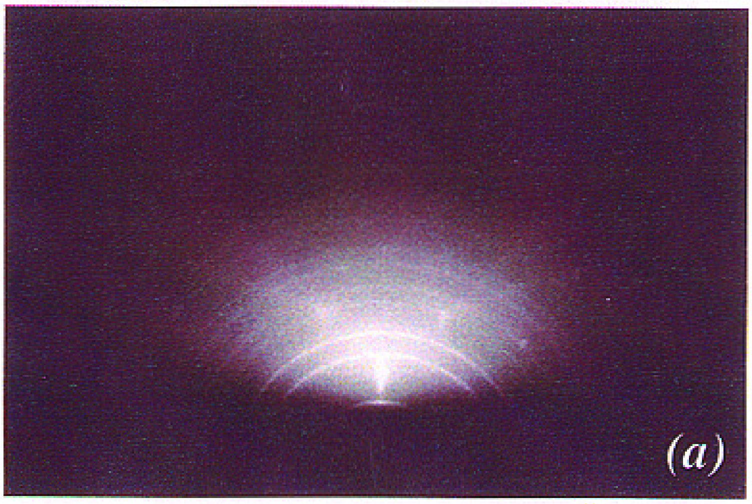
excitation source 350 nm
resolution 0.5 nm

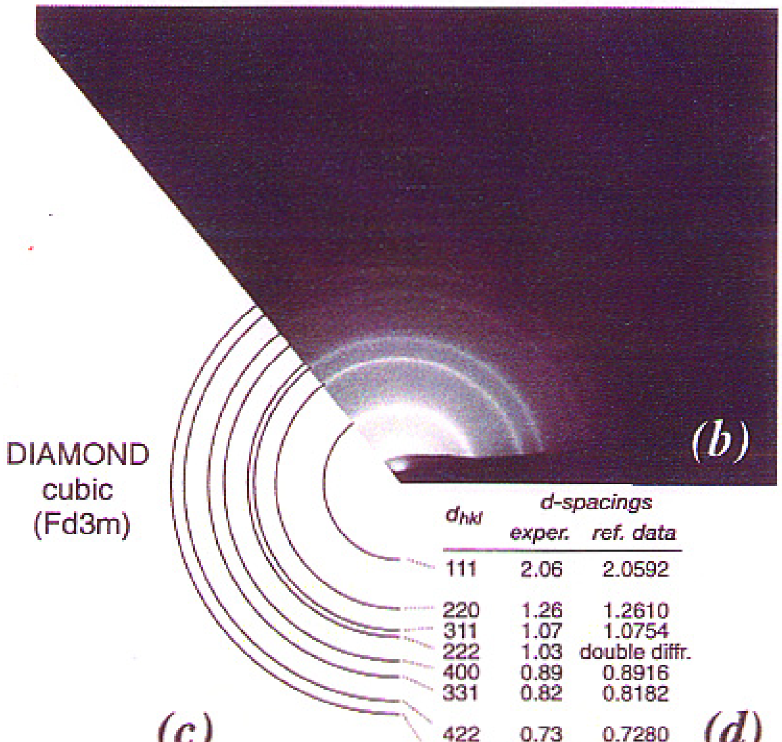
-Electron Spin Resonance

frequency	9.4 GHz
modulation	100 kHz
T	30- 300 K


1
2
3
4
μ

and THE CORRESPONDING STRUCTURES



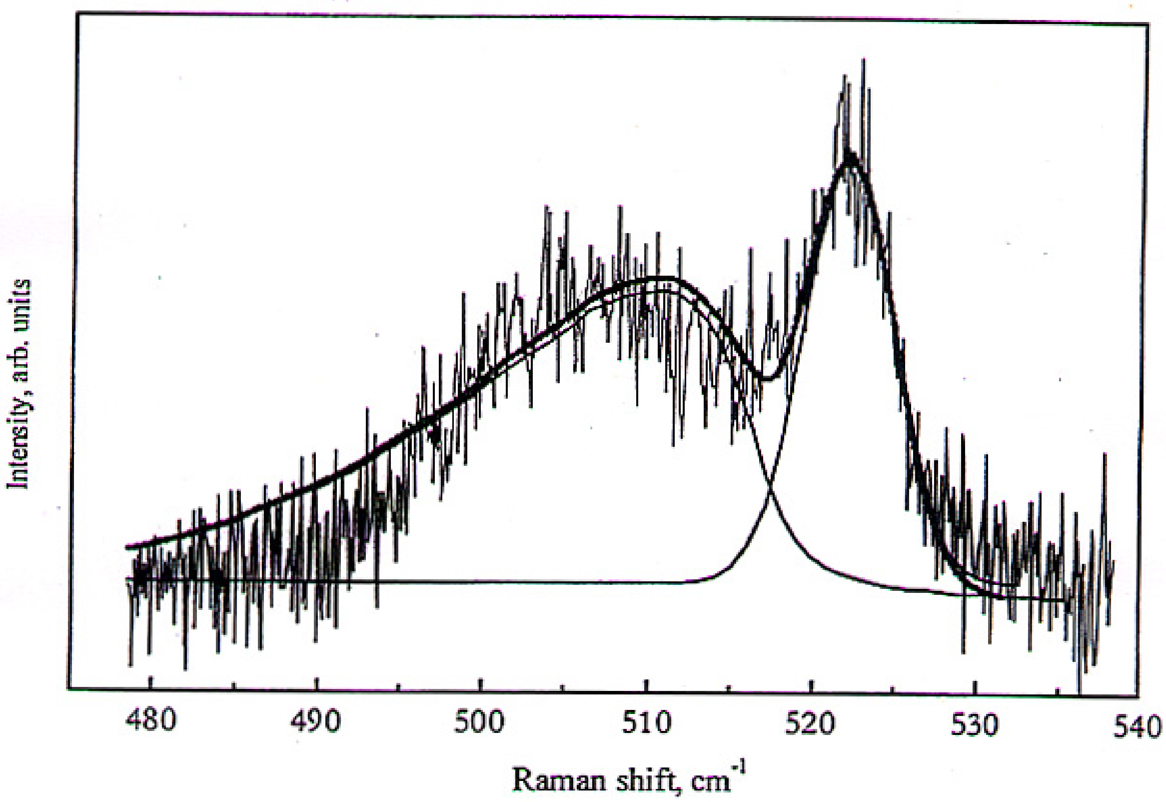


(c)

d_{hkl}	d-spacings exper.	d-spacings ref. data
111	2.06	2.0592
220	1.26	1.2610
311	1.07	1.0754
222	1.03	double diffr.
400	0.89	0.8916
331	0.82	0.8182
422	0.73	0.7280
511-333	0.68	0.6864

(d)

Raman spectrum of the Si-region

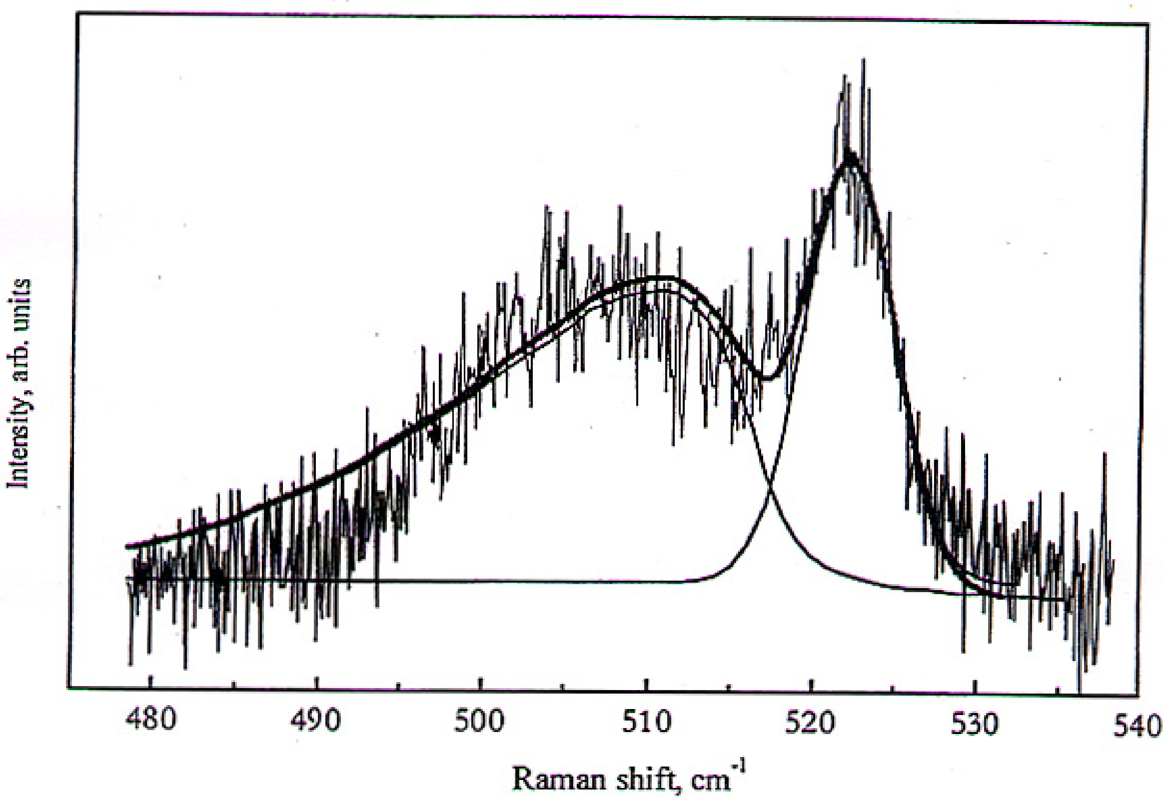


Raman peaks :

510 cm^{-1} (FWHM : 18 cm^{-1})

522 cm^{-1} (FWHM : 5 cm^{-1})

Raman spectrum of the Si-region



Raman peaks :

510 cm^{-1} (FWHM : 18 cm^{-1})

522 cm^{-1} (FWHM : 5 cm^{-1})

Evaluation of the crystallite size

$$I(\nu) = \int \exp\left(-\frac{q^2 D^2}{16\pi^2}\right) \frac{d^3 q}{(\nu - \nu(q))^2 + (\Gamma_0/2)^2}$$

D: average diameter of the Si nanoparticles.

Γ_0 : half-width of the phonon band in c-Si

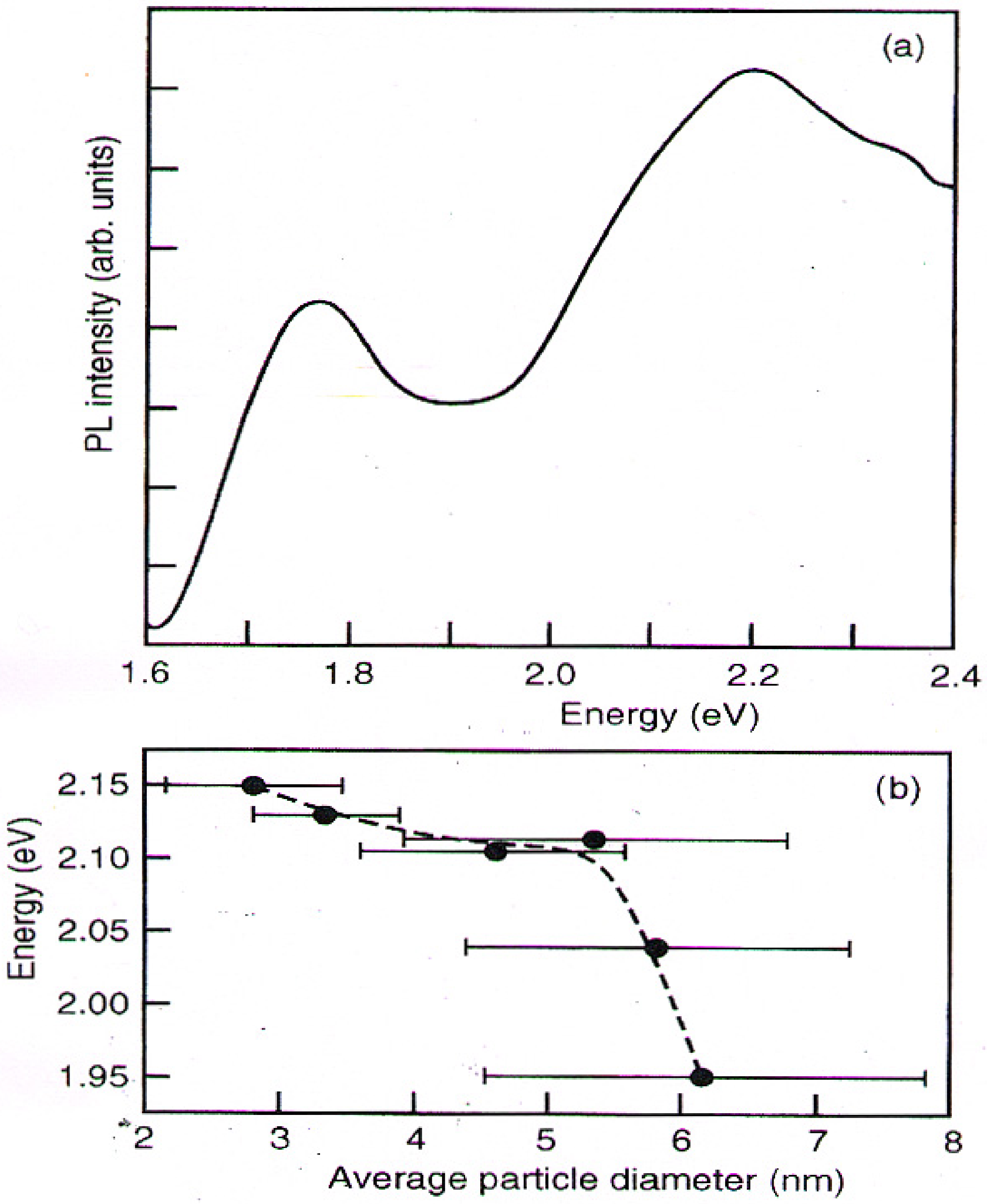
$$\nu^2(q) = A + \sqrt{A^2 - B(1 - \cos(qa))}$$

A= 1.36242 10^{15} cm^{-2}

B=8.47461 10^{19} cm^{-2}

$$\Downarrow$$

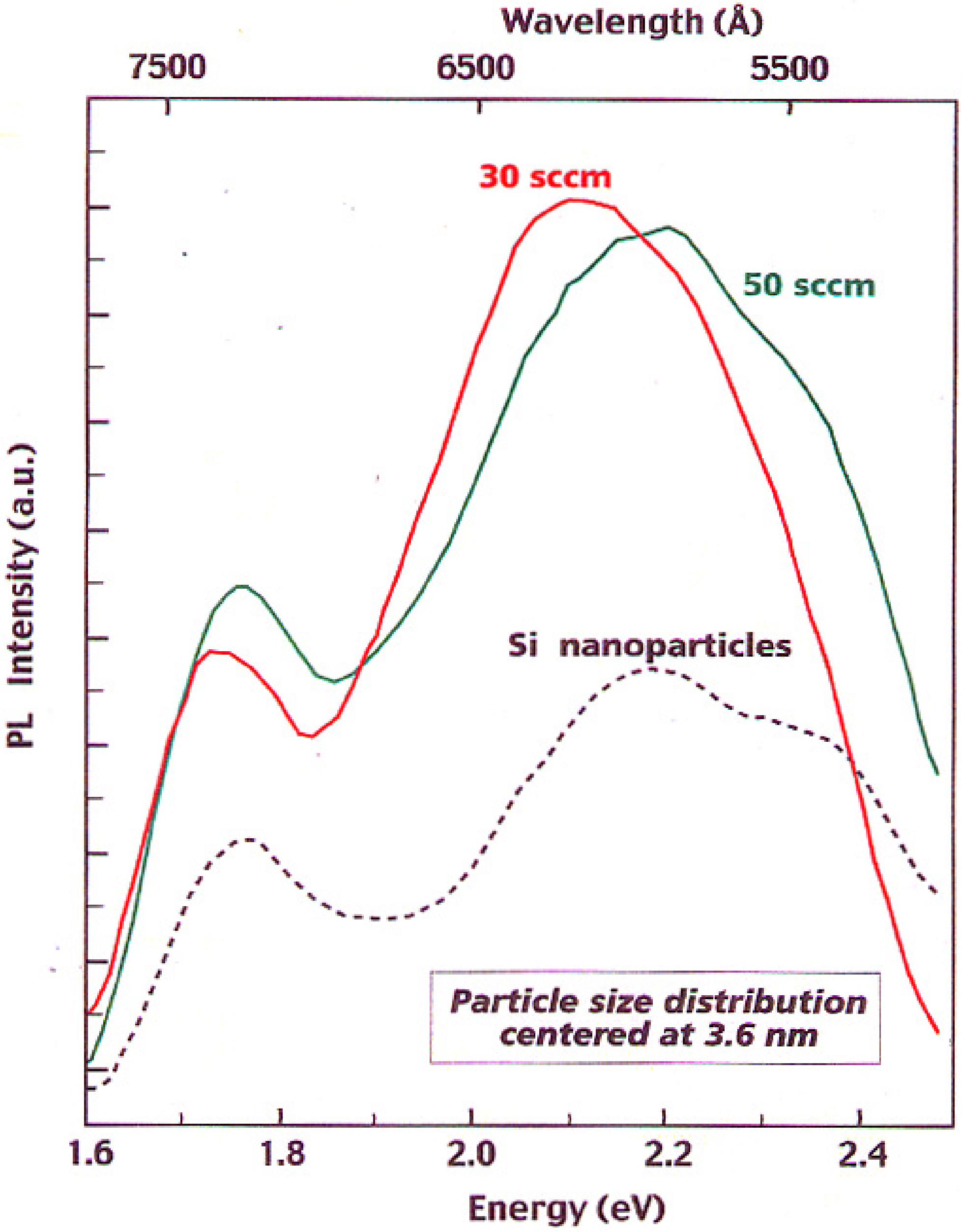
$$D \quad \cong \quad 3 \quad nm$$



(a) Room temperature emission of nanosilicon with <d> = 3.2 nm.

(b) Average energy of silicon nanoparticles emission band vs. average diameter.

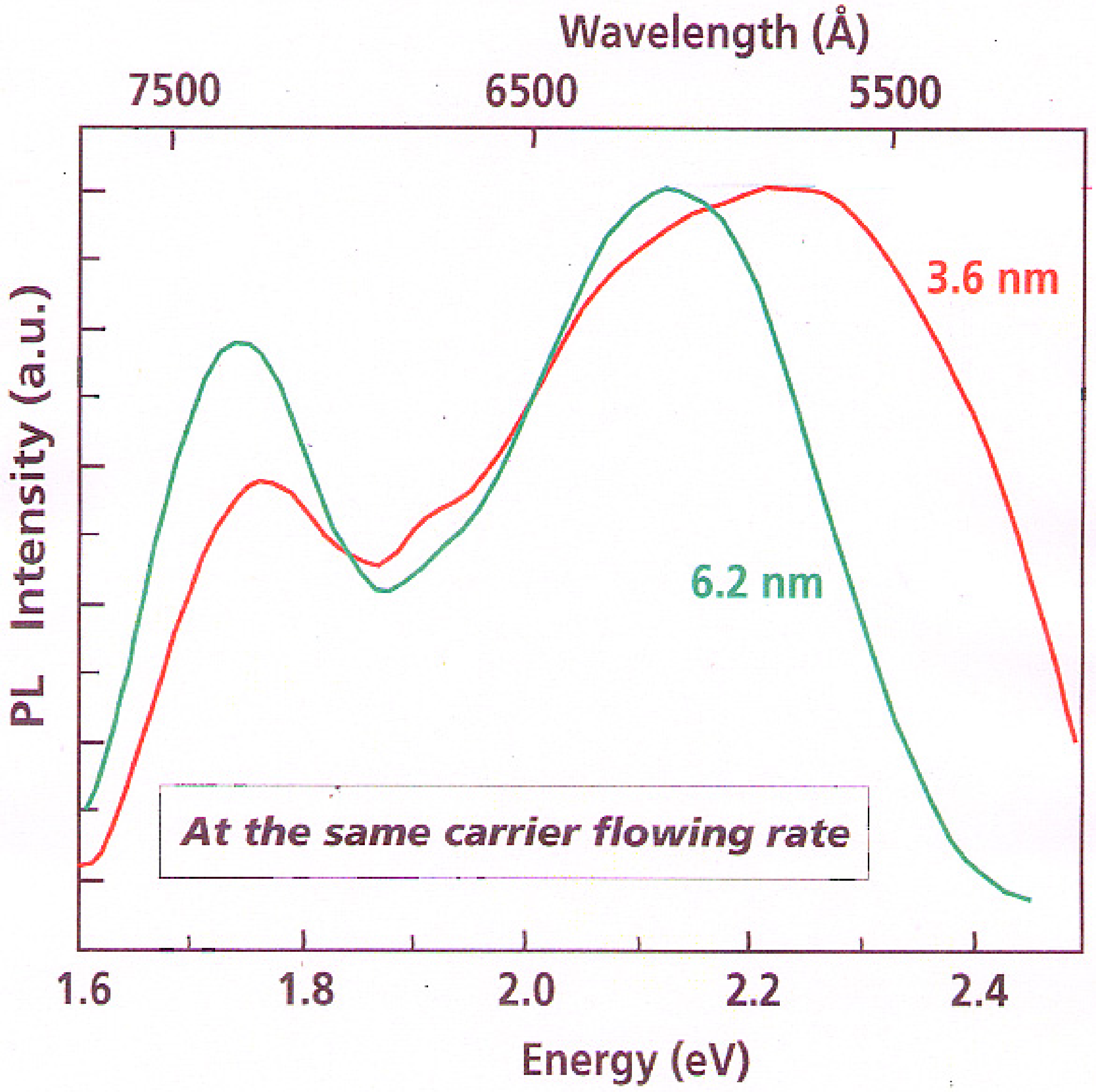
THE EFFECT OF THE CARRIER FLOWING RATE...

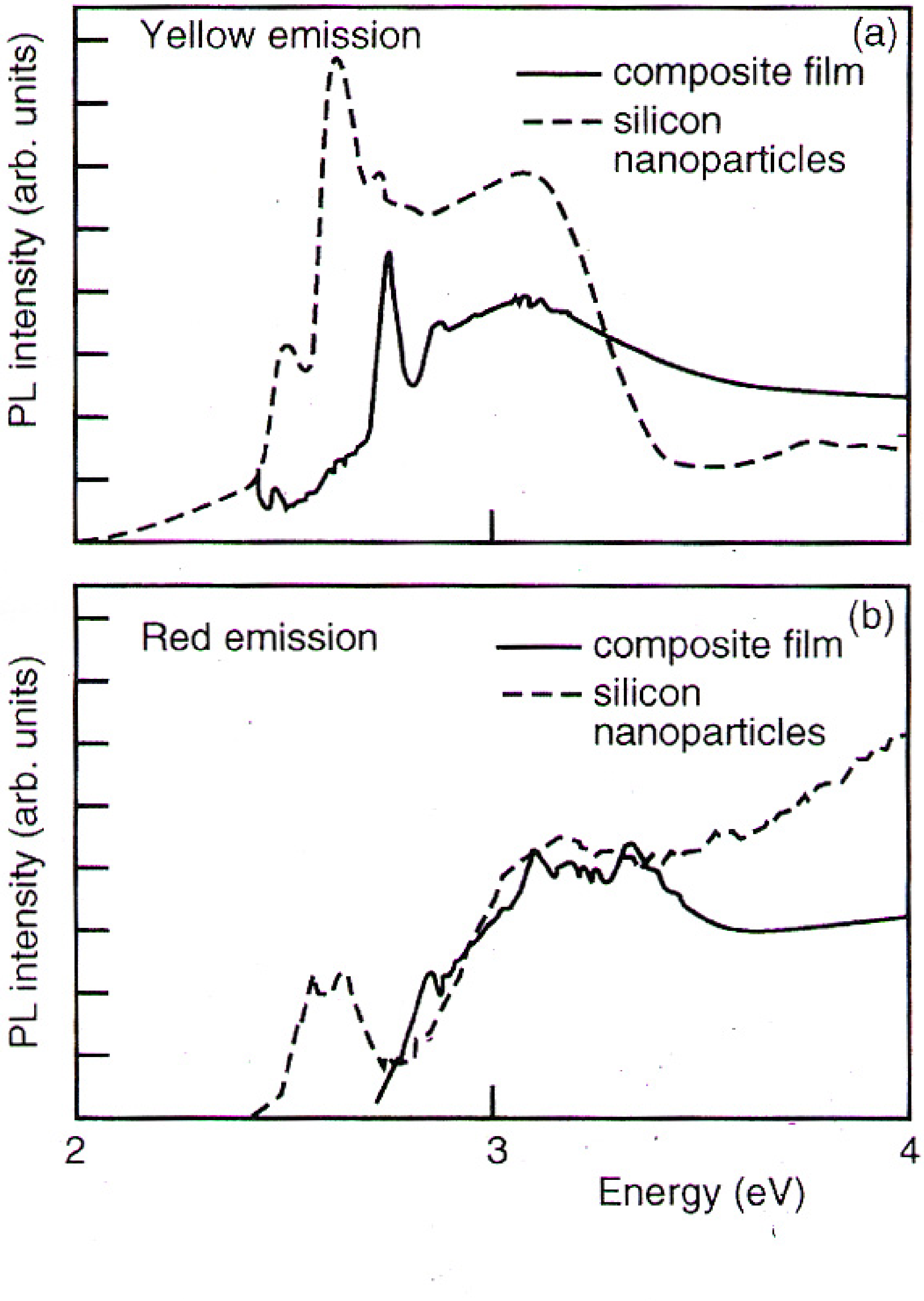


~ 1.7 eV

~ 2.0 – 2.2 eV

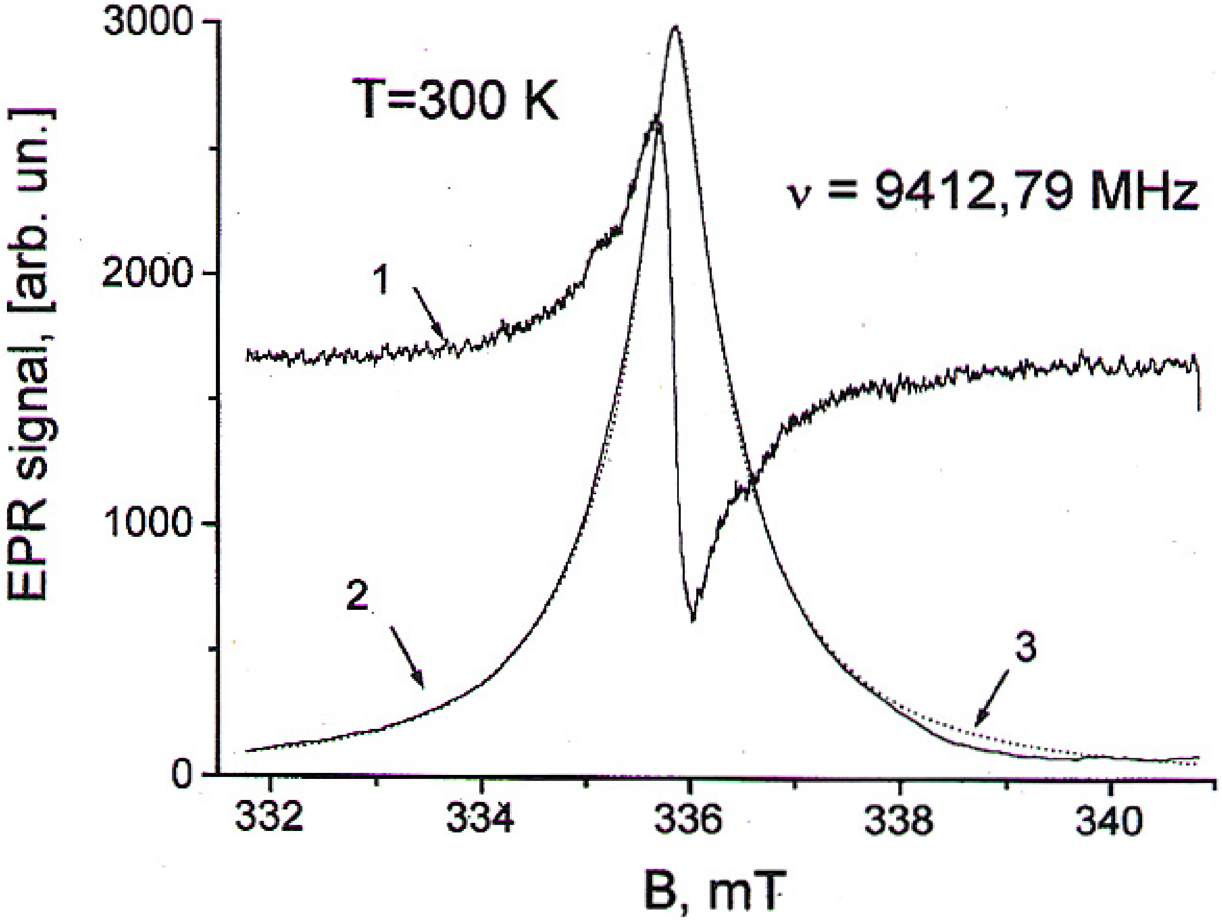
THE EFFECT OF Si PARTICLE SIZE





Excitation spectra of yellow and red emissions from silicon nanograins and composite films with <d> = 3.2 nm.

ESR spectra



Concentration of Paramagnetic Centers

$N = 4 \times 10^{19}$ cm^{-3}

Factor of Spectroscopic Splitting

$g = 2.0025 \pm 0.0001$

Full Width at Half Maximum of curve 2

to

Peak to Peak line-width of curve 1

$$\Delta H_{1/2} \,/\, \Delta H_{p-p} \approx 3$$

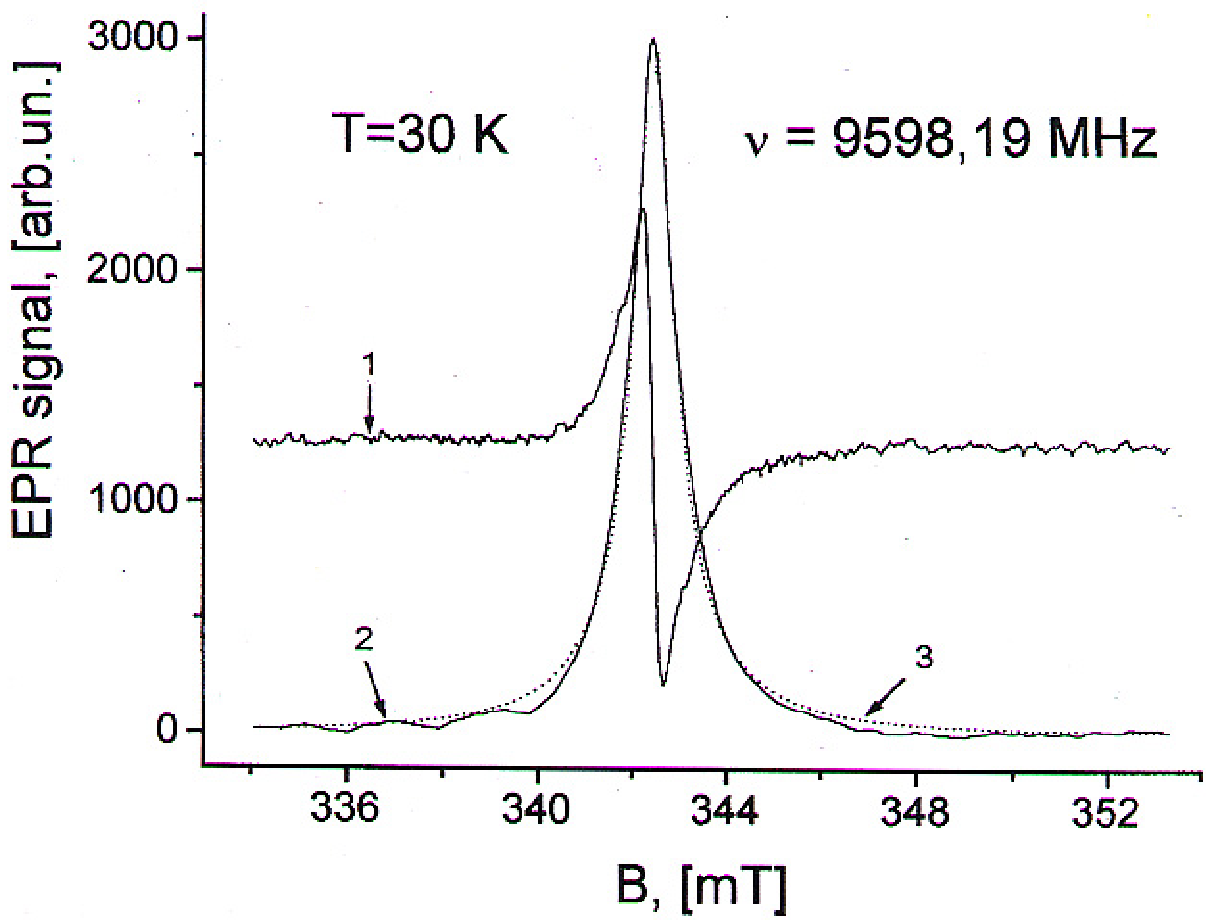
for a Gaussian line : 1.18
for a Lorentzian line : 1.73

Yper-lorentzian curve

The dotted curve is the sum of 3 Lorentzian curves :

$\Delta H_{1/2}$ = 5.4 G (0.37) - 12.6 G (0.36) - 24 G (0.27)

ESR spectra



T=30 K
ν = 9598,19 MHz
EPR signal, [arb.un.]
B, [mT]
3000
2000
1000
0
336
340
344
348
352
1
2
3

-The composite systems consist of Si quantum-dots inhomogeneously dispersed inside a polycrystalline diamond matrix

-The concentration of active centers (C) suggest a concentration of inserted Si quantum-dots of the order of 10^{19} cm^{-3}

-The average size of the inserted Si nanoparticles is of about 3 nm

-The crystalline quality of the diamond phase is not perturbed by the Si inclusion

-The emission properties are dominated by the Si quantum dots and the photoluminescence peak due to quantum-confinement effects is sensitive to the particle size

-The intensity of the room temperature emission from embedded Si quantum-dots is enhanced with respect to emission from the starting Si nanoparticles

-The emission properties of the inserted Si nanoparticles are stable and do not suffer from environmental degradation.

CONCLUSIONS

COMPOSITE CVD DIAMOND FILMS WITH PROPERTIES OF PHOTOLUMINESCENCE

- A new technique utilizing a powder-flowing apparatus coupled with a CVD reactor has been used to produce nanocomposite Si-containing diamond layers.

- The reported findings indicate that by acting on the flux rates it is possible to influence at the same time:
  - • the dispersion of Si-nanoparticles inside the matrix
  - •• the growth rate of the diamond phase

Overall, it is possible:

- *to modulate RT emission*
- *to enhance luminescence efficiency*
- *to control the crystalline quality of the diamond matrix*

by inserting Si powders with suitable grain sizes

by operating grain size selection flowing the carrier at selected flux rates