

Boron-Interstitial Clusters (BICs)

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IMPORTANCE of BICs

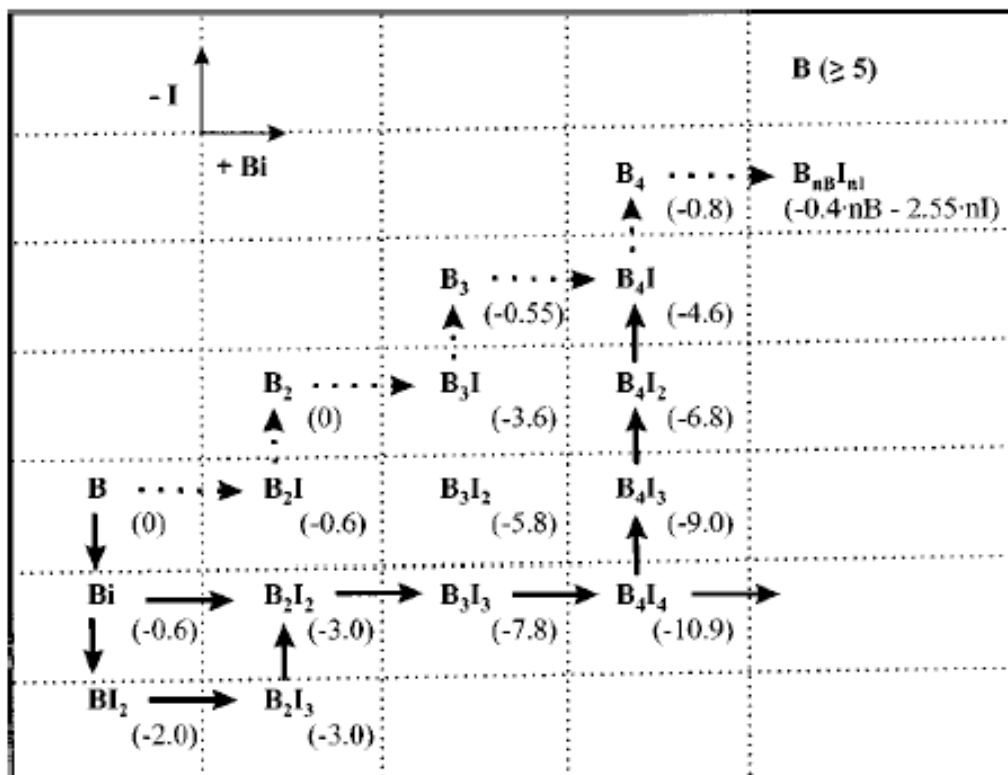
Production of ultra-shallow boron implants with high activation rate requires tight control of the post-implantation annealing.

- Self-interstitials, created by the radiation damage, mediate fast transient diffusion of boron, during which stable and metastable BICs are formed.
- BICs decrease the activation rate.



MODELING OF ANNEALING KINETICS

- Simulation of BIC evolution with formation energies as parameters to fit SIMS profiles [e.g. Pelaz et al. APL 1999]



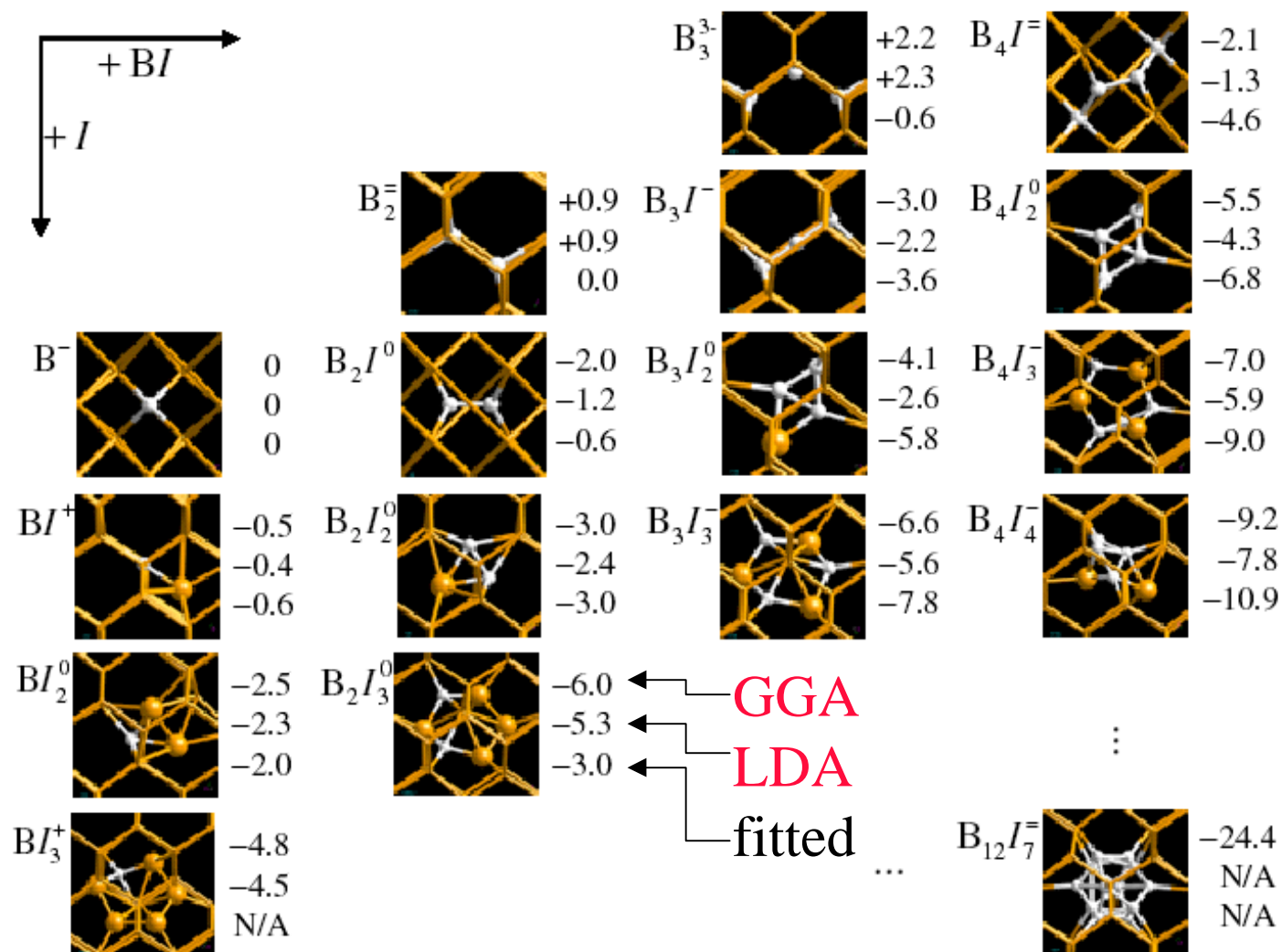
-too many parameters!
 -what is the activation rate?



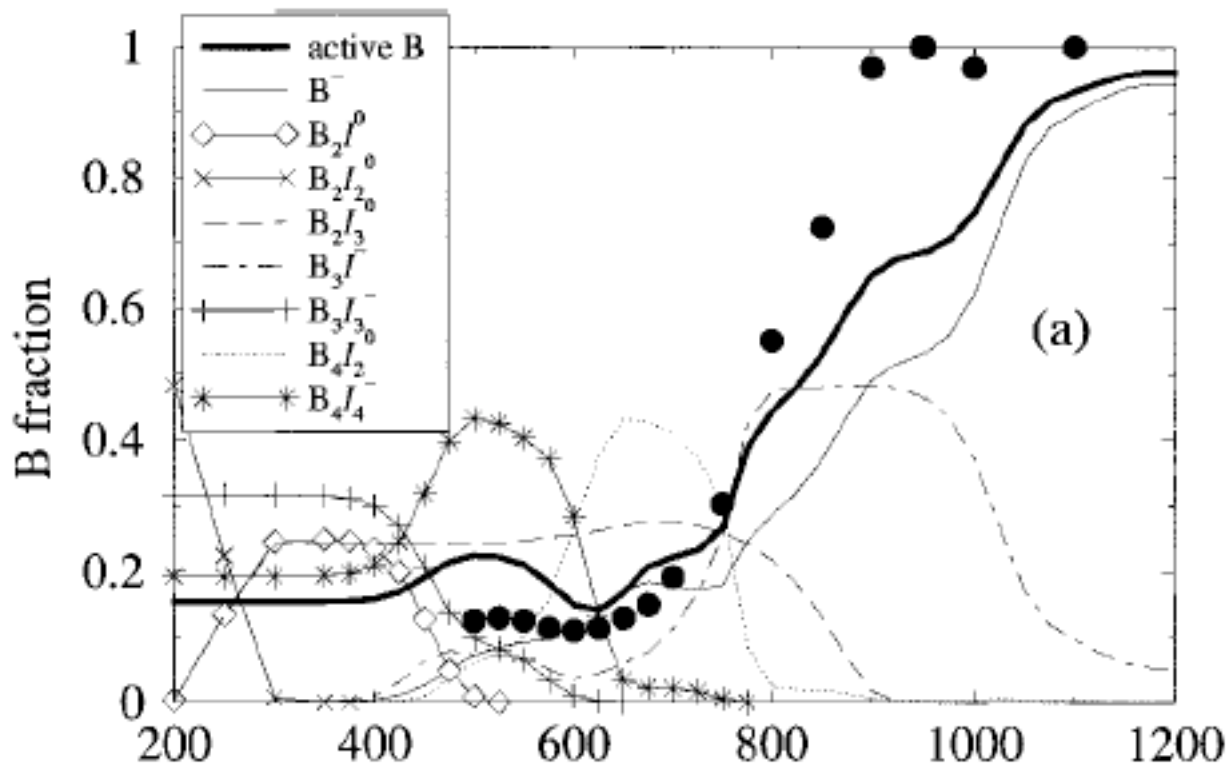
INPUT from *AB INITIO*
 defect calculations

GGA and LDA
 calculations

[Windl et al.
 APL 2000]



W. Windl, X.-Y. Liu & M.P. Masquelier, Phys. Stat. Sol. (b) **226**, 37 (2001)



Fraction of B atoms trapped in the different clusters (GGA).

“Active B” sums up all holes provided by isolated and clustered B.

Experimental data are shown by dots.

WHAT'S THE PROBLEM?

W. Windl, X.-Y. Liu & M.P. Masquelier, Phys. Stat. Sol. (b) **226**, 37 (2001); Appl.Phys.Lett. **77**, 2018 (2000) — *the MOTOROLA group*

- *“We want to point out that despite the fact that GGA and LDA predict somehow comparable energies and activation behavior ..., the clustering paths are substantially different.”*
- *“The differences, in conjunction with the different levels of corrections, add up to large differences in most of the reaction barriers between our work and Ref. [14], up to more than 1 eV.*

[14] T.J. Lenosky, B. Sadigh, S.K. Theiss, M.J. Caturla, T. Diaz de la Rubia, Appl.Phys.Lett. **77**, 1834 (2000). — *the LIVERMOORE group*

Conclusion: too many different BIC formation energies with relatively high error bar does not help much in understanding the kinetics!

Objective of our research:

let's **identify the key players first directly by** means of the combined use of **experiment** (IBA + vibration spectroscopy + electrical measurements) **and theory** (calculation of equilibrium geometry + vibration modes + occupation levels)!

EXPERIMENT: **earlier** IR, DLTS, EPR **only** on compensated samples e-irradiated at low T and annealed up to 300 °

THEORY: **ready to go** (while samples are prepared and experiments set up)

COMP. CODE	Model	Hamiltonians	Basis for ψ	Ionic core	Purpose
SIESTA 1.1	64,216 supercell 2 ³ MP	GGA	Numeric AOs i double $\zeta+d$ FFT: 90 Ry	Norm conserv. PP	geometry vibrations
CRYSTAL'98	64 atom supercell 2 ³ MP	LDA with 20% exact exch.	ECP-21*G 6-21*G (AE)	Norm conserv. PP or All-Electron	levels hf tensor

CONVERGENCE TESTS: Si:V₂ the correct geometry is obtained with a 216-atom SC and does not change for 512 and 1000. Consequently BICs were tested in 64 and 216 supercells.

Windl

	64 (1)	64 (2 ³)	64, (4³)	216, (2 ³)	216, (1)
I	2.53	3.65		3.61	3.35
B ⁻	-80.33-μ _B	-80.46-μ _B		-80.53-μ _B	-80.50-μ _B
BI ⁺	-0.24	-0.69	-0.5		-0.42
BI ₂	-2.14	-2.30	-2.4		
B₂²⁻	+0.87	+0.76	+0.9		+0.88
B ₂ I	-1.07	-1.71	-1.7		-1.44
B ₂ I ₂	-1.98	-2.74	-2.7	-2.53	-2.35
B ₃ I ⁻	-1.98	-2.67	-2.7		-2.30
B ₄ I ²⁻	-1.31	-1.92	-2.1	-1.66	-1.53

Cluster geometries identical to 0.01 Å in 64 and 216 atom calculations.
 Vibrations were calculated in 64. Values given for ^{11}B (^{10}B) in [cm^{-1}].

	64, 1 MP			64, 2 ³ MP
	All atoms	3 NN	2 NN	2NN
B_5^-	610(634)	609(634)	610(634)	607(632)
B_2^{2-}	618(647) 590(615)		618(647) 589(617)	627(657) 577(602)
B_2I_2		880(921) 669(694) 575(595) 556(577)	880(920) 670(696) 576(597) 554(575)	926(969) 684(710) 565(585) 539(560)
$\text{B}_4\text{I}_2^{2-} (\text{C}_{2v})$		961(1008) 771(809) 727(756) 655(683) 643(669) 606(633)	961(1008) 771(809) 729(758) 657(685) 642(668) 607(634)	1019(1068) 744(780) 730(759) 652(679) 641(667) 609(637)

Results in [cm⁻¹] for ¹¹B (¹⁰B) from 64-atom cell with 2NN :

B_s^-	B^-	T_2 (IR/R)	607(632)		
B_i^+	BI^+		< 520		
$(B_s + Si_i)^+$	BI^+	A_1 (IR/R)	693 (723)		
$((B + Si)_s + Si_i)^-$	BI_2^-	A' (IR/R)	671 (698)	A'' (IR/R)	658 (684)
$(B_s)_2^0$	B_2^0	A_{1g} (R)	644(674)	E_u (IR)	527(547)
$(B_s)_2^{2-}$	B_2^{2-}	A_{1g} (R)	627(657)	E_u (IR)	577(602)
$(B_2)_s^0$	B_2I^0	A_1 (R)	1099(1152)	E (IR,R)	738(767)
$(B_s - Si_i - B_s)^0$	B_2I^0	A_{1g} (R) E_g (R)	672(706) 586 (608)	A_{2u} (IR) E_u (IR)	882(908) 604(628)

Results in [cm⁻¹] for ¹¹B (¹⁰B) from 64-atom cell with 2NN and (2³) MP set:

$(B_s - Si_i - B_s)^=$	$B_2I^=$	A' (IR/R)	821(852) 666(692) 573(594)	•A''(IR/R)	719(748) 582(604) 569(589)
$[(B_2)_s + Si]^0$	$B_2I_2^0$	A' (IR/R)	926(969) 565(585)	A''(IR/R)	684(710) 539(560)
$(B_s + B_i + B_s)^-$	B_3I^-	A _{2u} (IR) E _u	1264(1326) 652(679)	A _{1g} (R) E _g	842(882) 612(635)
$(B_s (B_2)_s B_s)^0$	B_4I^{2-}	A'(IR/R)	1095(1148) 729(763) 639(665) 566(589) 564 (587)	A''	814(853) 637(663)

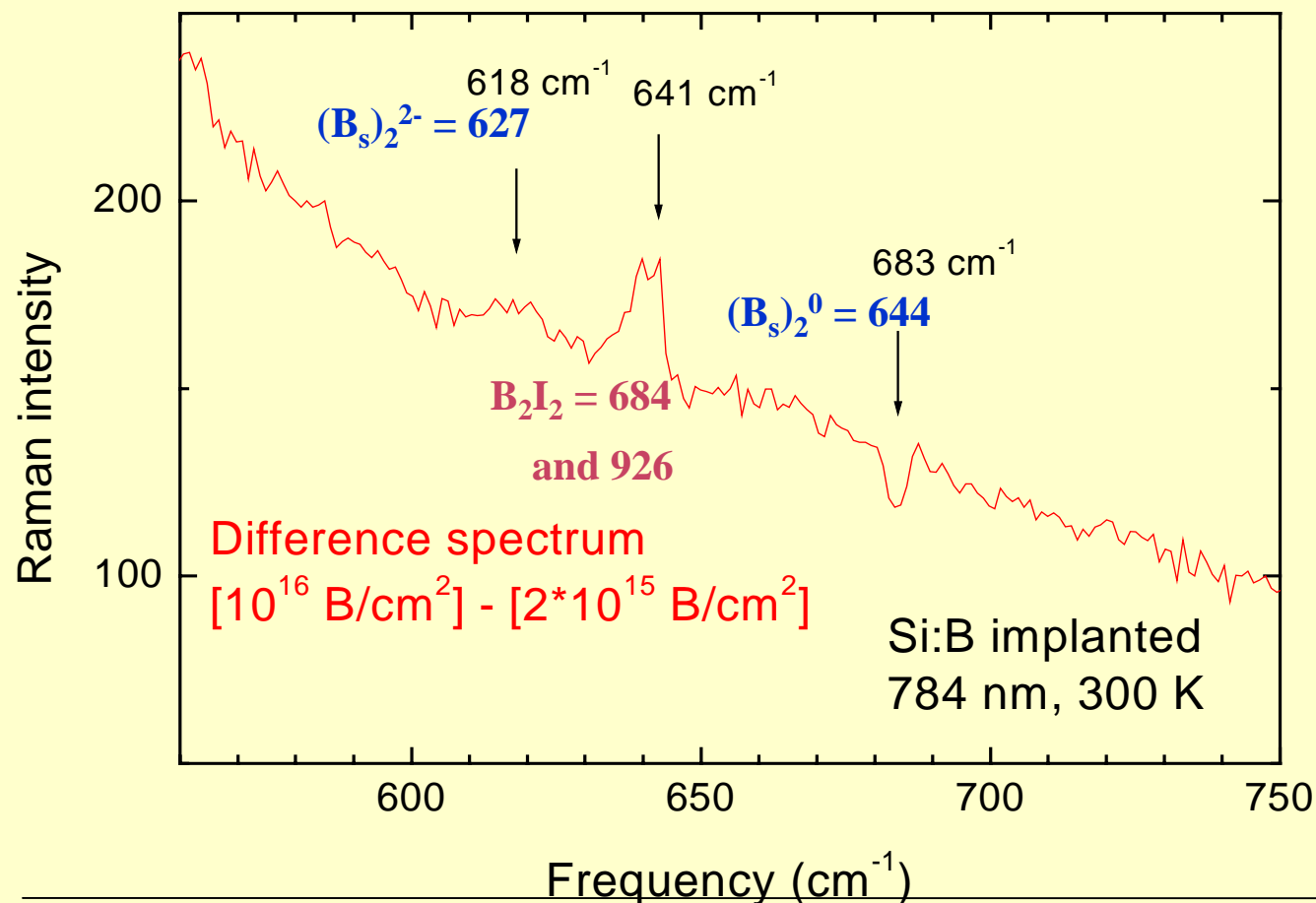
Modes of mixed isotope combinations are also available!

FRENDTECH WORKSHOP
Erlangen, February 11,2003

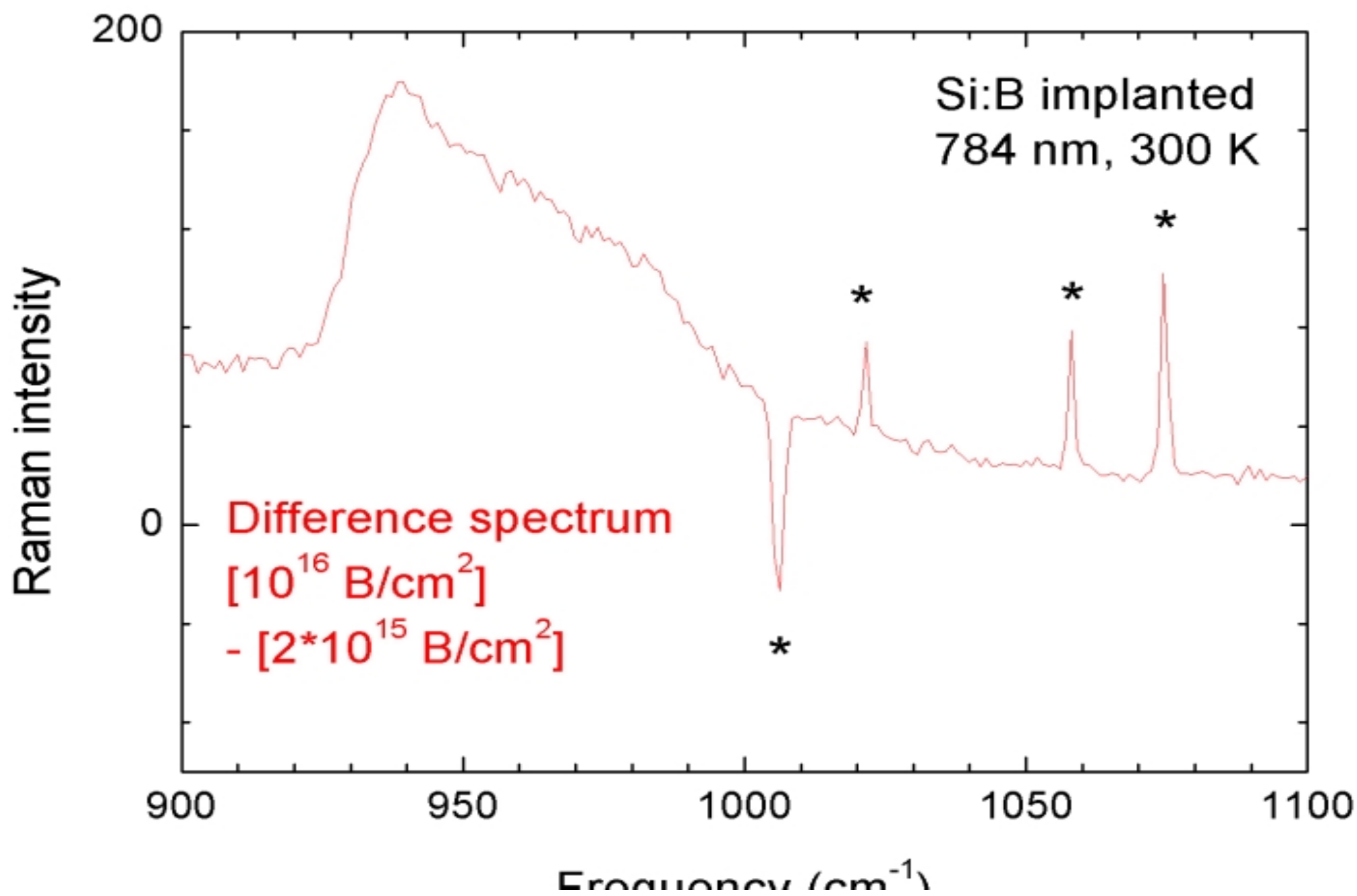
Early expts on *e*-irradiated compensated Si or after *n*-irrad. and annealing:

Center	accep -tor	R-lines < -40C	S-lines -40 ---10C	Q-lines -10—220C	P-lines surv>300C	I2 center app. ~200C
Expt.mode	623	730	903, 599	733	553	843, 242
Assign.	B_s^-	B_i+nSi_i	2B with C_{3v}	B_i	$(B_s)_2$	$2B_s+Si_i$
Model	B_s^-	$(B_s+Si_i)^+ ?$ $(B_s+2Si_i)^- ?$	$B_s+Si_i+B_s?$	$(B_2)_s$	$(B_s)_2 / (B_s)_2^{2-}$	Si_i $B_s^- \quad B_s^- ?$
Yamauchi (theory)	T_2 612			A_1 1026 E 760	E_u 530 A_{1g} 585 E_g 603	
PRESENT (theory)	T_2 607 ↑ E-BAR	A_1 691 NO A_1 671 NO	A_{2u} 882 A_{1g} 672 E_u 604 E_g 586 YES	A_1 1031 E 748 YES	E_u 527/577 A_{1g} 644/627 YES	821 ??? 719 666 582 573 569

New Raman meas. On ^{11}B -implanted samples after 900 C anneal.
Difference on increasing dose from $2 \cdot 10^{15}$ to 10^{16} cm^{-2} .



Higher dose
↓
more damage
↓
higher compensation
↓
higher E_F
↓
more $(\text{B}_s)_2^{2-}$ and
less $(\text{B}_s)_2^0$



CONCLUSION

- **hope** seems to be justified for identification of key BICs at different T
- **fun**: the two BICs (possibly) seen so far did not figure high in earlier simulations!

Acknowledgment:

Peter Pichler and **István Bársony** for initializing and counseling this work

P.P. & Alan Claverie for providing supercomputer time

HLR Stuttgart, CRAY T3E 40 kSU/year courtesy of FhG-IIS-B

NISC Jülich, CRAY T3E 20 kSU/year, courtesy of FhG-IIS-B

CINES Montpellier, IBM SP3 20 kSU/year, courtesy of CEMES/CNRS
