

Anti-Phase-Boundary Defects in GaAs-on-Si Films:

1. characterization by SHG
2. suppression by ART

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The microelectronics industry is trying to marry III-V and Column IV semiconductors via hetero-epitaxy to combine the favorable properties of each

High mobility FETs (Intel 2009)

Metal gate electrode

InGaAs

Si

High-K/InP composite gate insulator stack ($t_{oxe} = 2.2\text{nm}$)

Efficient solar cells

>50%

HighGap

InGaP

GaAs

Si

LowGap2

Ge

40%

InGaP

GaAs

Ge

~15%

Si

~30%

GaAs

single junction

multi-junction

III-V nanolasers on Si

GaAs shell

InGaAs core

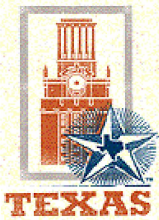
Si

Chen, *Nat. Phot.* **5**, 170 (2011)

Tilt view

c-axis

500 nm



GaAs/Si interfaces are susceptible to formation of defects

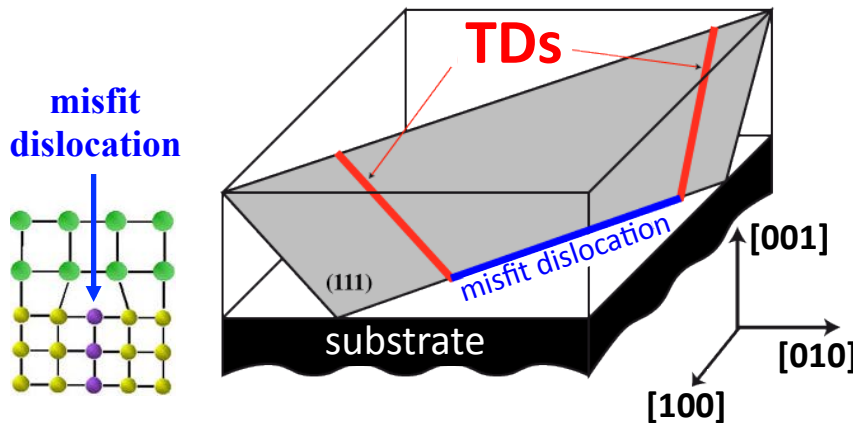


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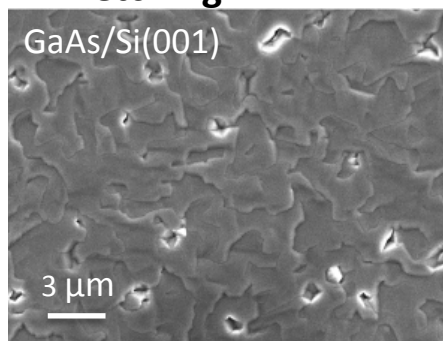
Threading Dislocations (TDs)

Where: any hetero-interface

Cause: lattice mismatch



Characterization: selective etching + TEM



Hsu, *Nanotech.* 23, 495306 (2012)

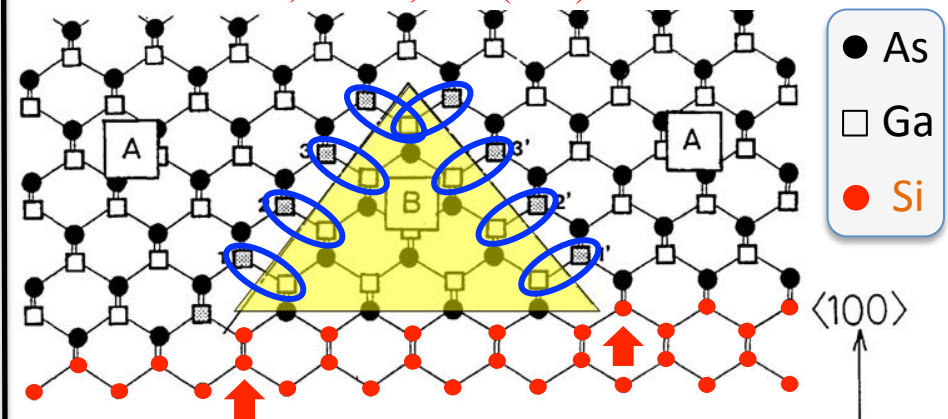
sub- strate	lattice mismatch w. GaAs	typical TDD [cm ⁻²]
Si (001)	4%	>10 ⁹
Ge (001)	<1%	<10 ⁸

Anti-Phase Domains (APDs)

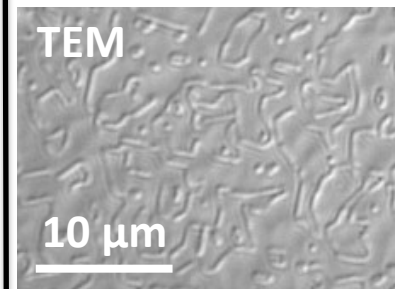
Where: polar-on-nonpolar hetero-interfaces

Cause: single-atom steps, nonpolar substrate (↑)

Kawabe, *JJAP* 26, L944 (1987)



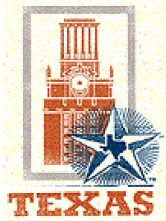
Ga-Ga bonds along **Anti-Phase Boundaries (APBs)** degrade carrier mobility



Brammertz, *TSF* 517, 148 (2008)

TDs and APBs are challenging to distinguish in TEM micrographs

To evaluate strategies for suppressing these defects, a fast, noninvasive diagnostic that clearly distinguishes APBs from TDs is needed

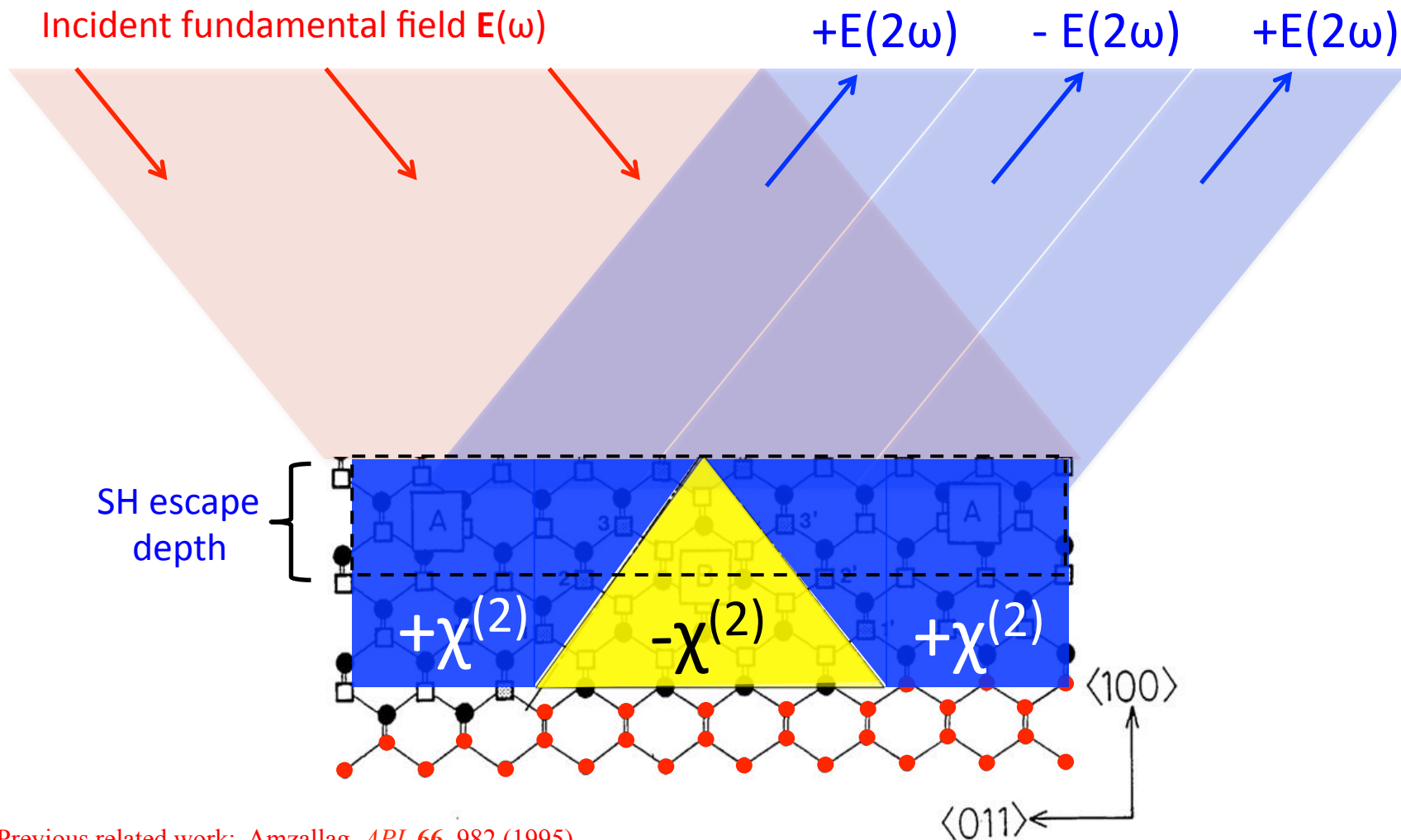


Neighboring APDs generate SH fields of opposite sign

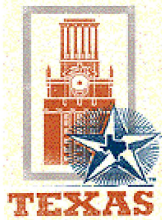


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Destructive interference in far field



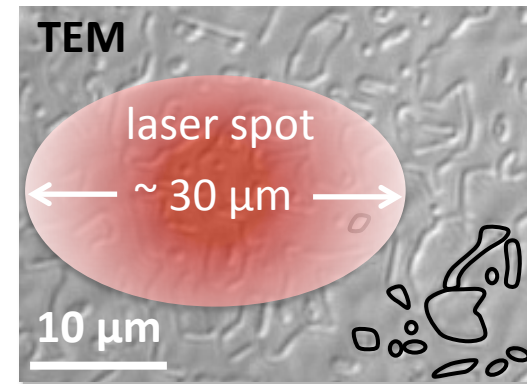
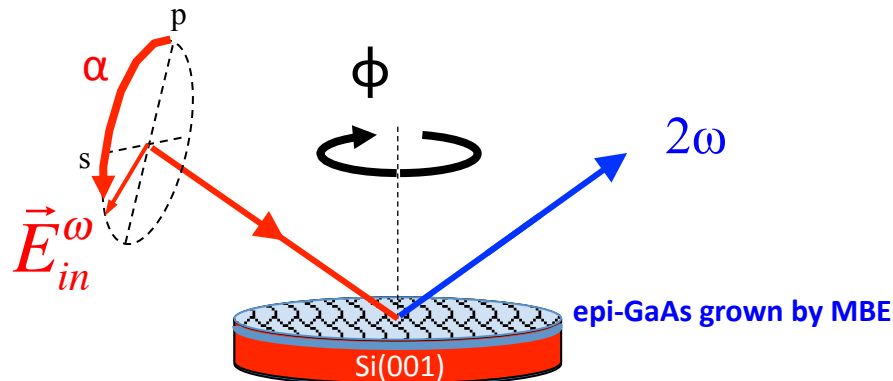
Previous related work: Amzallag, *APL* 66, 982 (1995)



SHG characterizes APBs sensitively and non-invasively

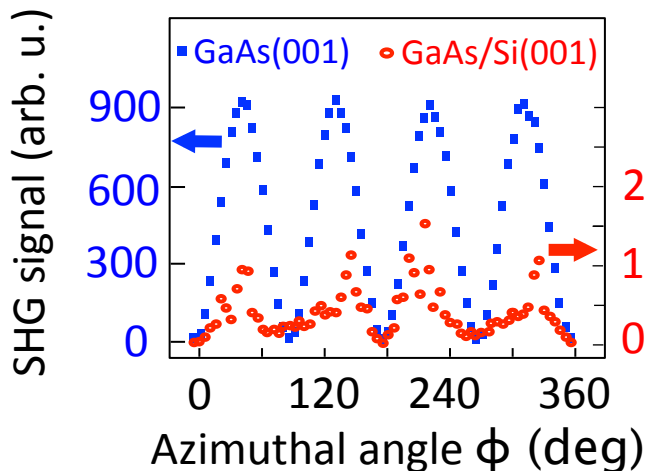


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APDs:
0.1 – 2 μm

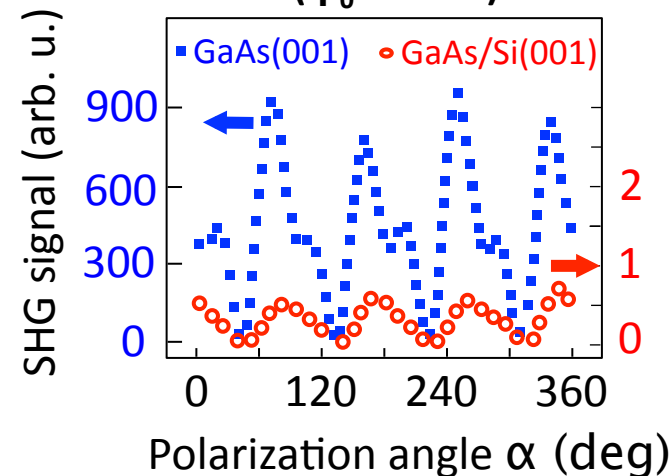
sample azimuthal rotation
(p-in/s-out)



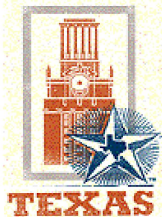
$$I_s(2\omega) \propto |\sin 2\phi|^2$$

[Yamada. *Phys. Rev. B* 49, 14372 (1994)]

incident polarization rotation
($\phi_0 = 22.5^\circ$)



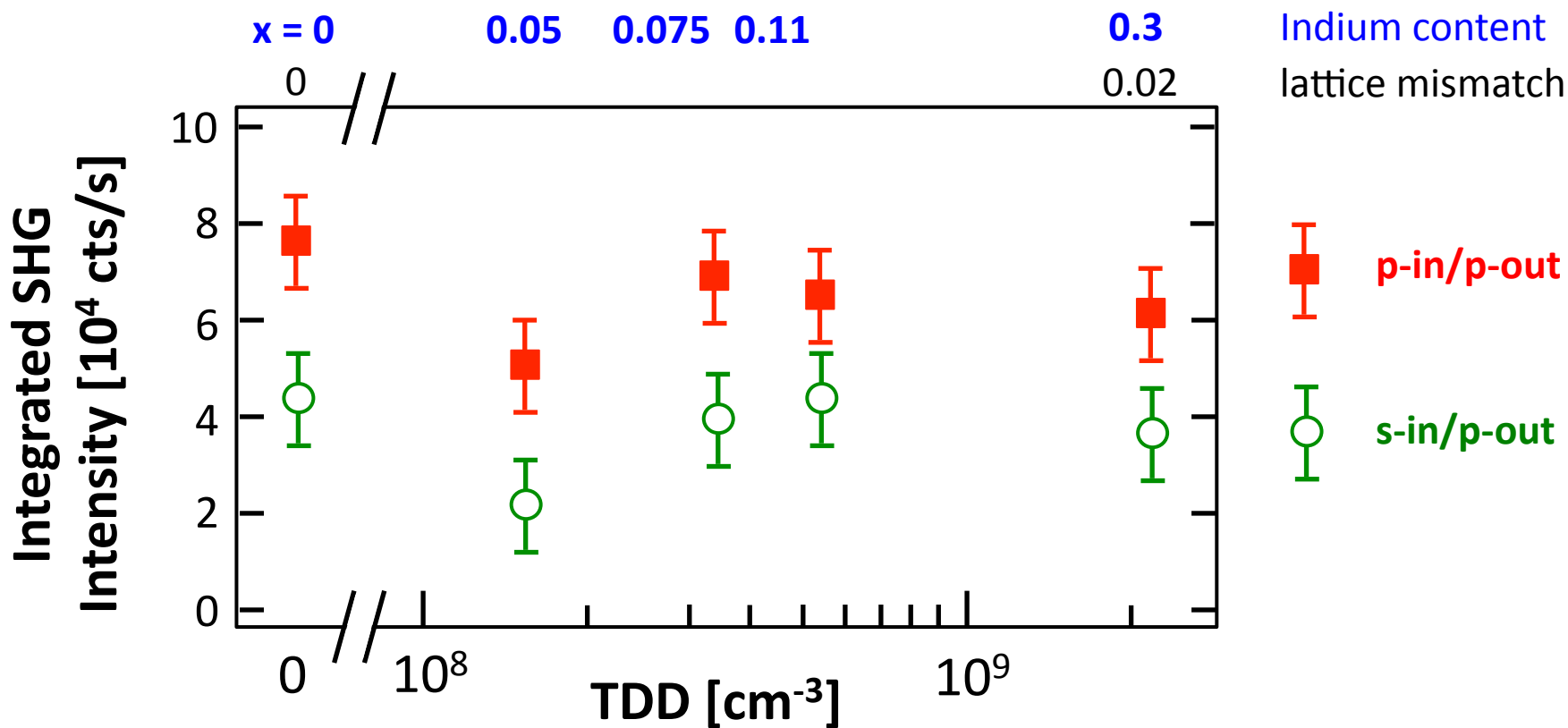
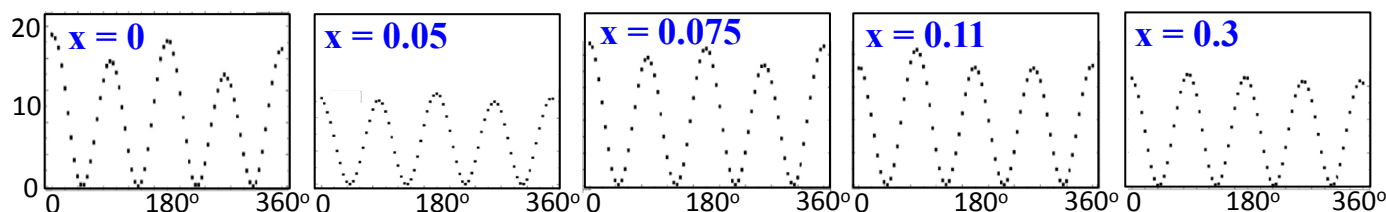
$$I_s(2\omega) \propto |\cos\alpha(f_c t_p \cos 2\phi_0 \cos\alpha + t_s \sin 2\phi_0 \sin\alpha)|^2$$



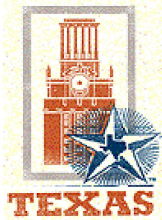
To test SHG sensitivity to TD Density (TDD), we prepared $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ samples



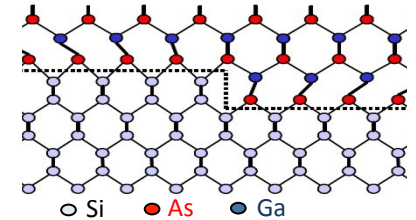
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Conclusion: SHG is uncorrelated with TDD

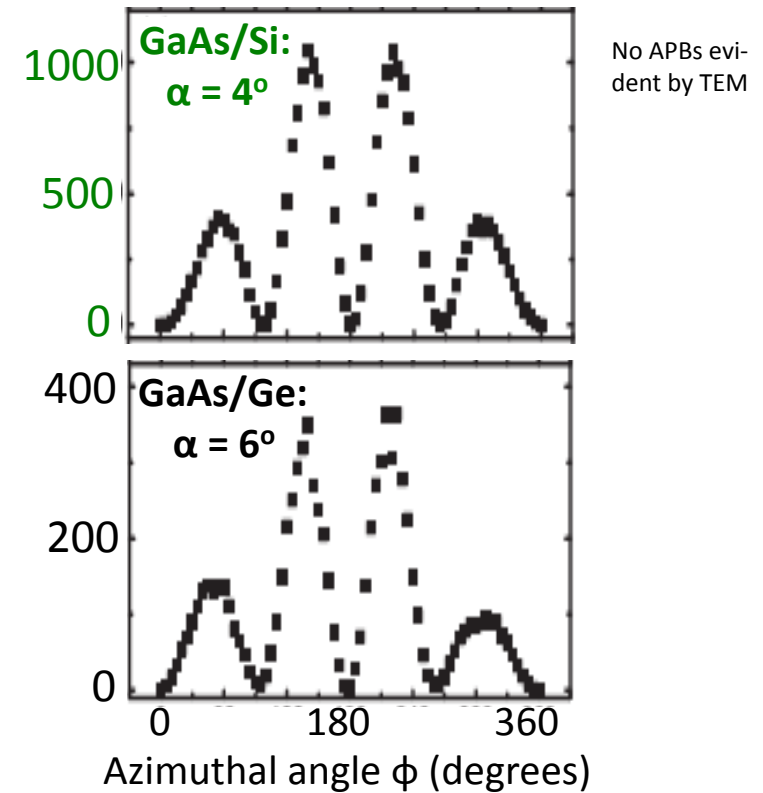
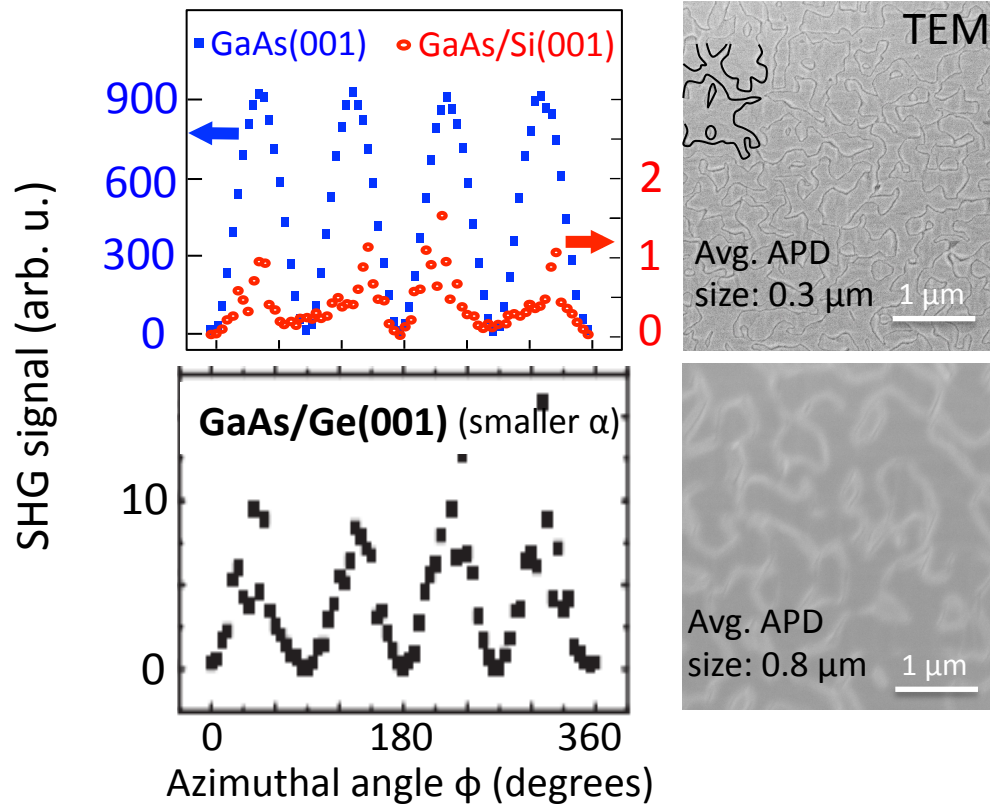


Substrate off-cut angle α strongly affects APD density & SHG suppression



$\alpha < 1^\circ$: single-atom steps dominate;
SHG suppression correlates with APD density

$\alpha \geq 4^\circ$: double-atom steps dominate;
APDs suppressed, SHG recovers

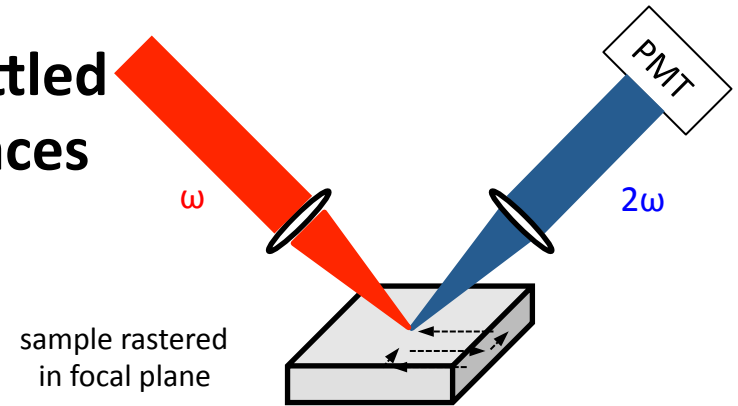


	GaAs	GaAs/Si(001)	GaAs/Ge(001)	GaAs/Si: 4°	GaAs/Ge: 6°
<SHG intensity>	1	2.4×10^{-3}	7.7×10^{-3}	0.74	0.24
Roughness nm	0.9	1.0	5.8	1.8	16
TDD /cm ⁻²	N/A	8×10^9	2.5×10^8	5.5×10^8	2.4×10^7

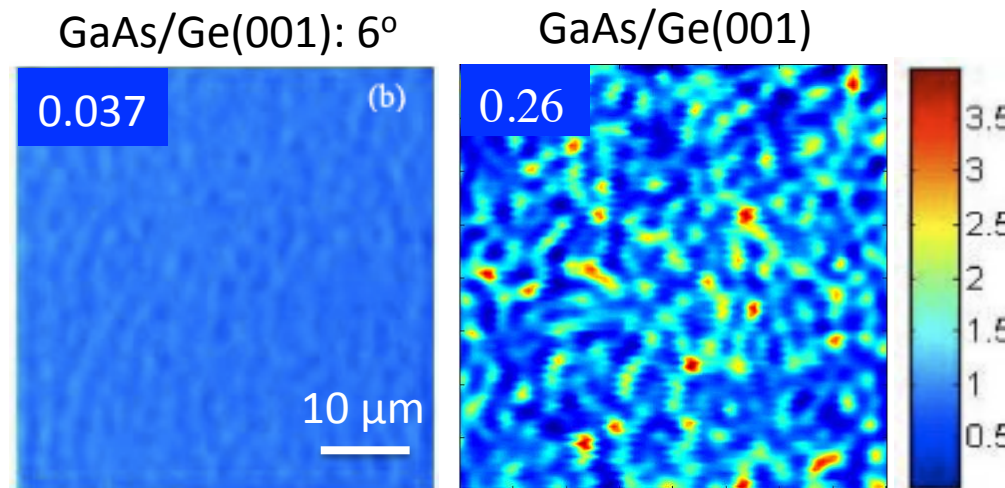
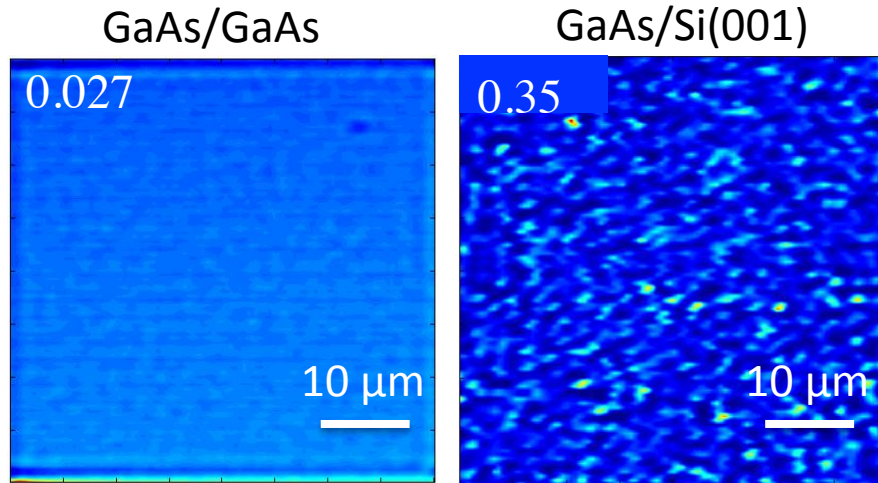


Scanning SHG microscope yields mottled SHG response from APD-laden surfaces

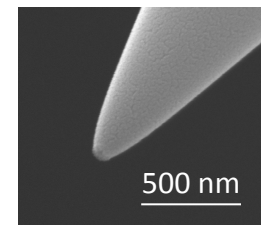
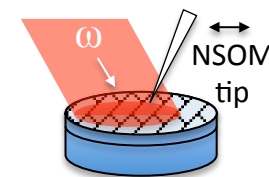
Lei et al., APL 102, 152103 (2013)



St. Dev. →
of SHG
intensity



- The SHG images are NOT direct maps, but rather higher-order moments, of the APD distribution.
- **Bright areas** indicate dominance of one type of domain within the laser spot.
- **Dark areas** indicate equal areas of $+\chi^{(2)}$ and $-\chi^{(2)}$ domains within the laser spot.
- **SHG NSOM*** may be able to image individual APDs directly.



*Smolyaninov, *Phys. Rev. B* **56**, 9290 (1997)
Bozhevolnyi, *Opt. Commun.* **150**, 49 (1998)



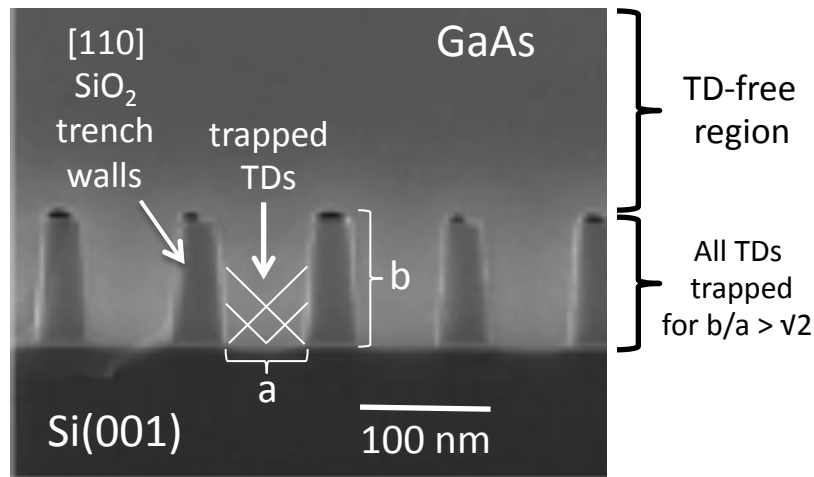
Growth of GaAs on exactly oriented Si(001) is preferred for high-volume manufacturing



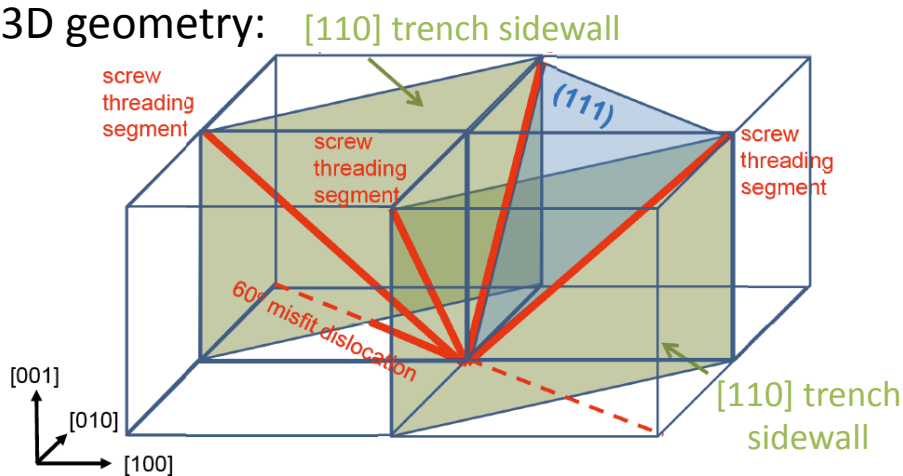
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Aspect-Ratio Trapping (ART) is an established technique for suppressing TDs on Si(001)

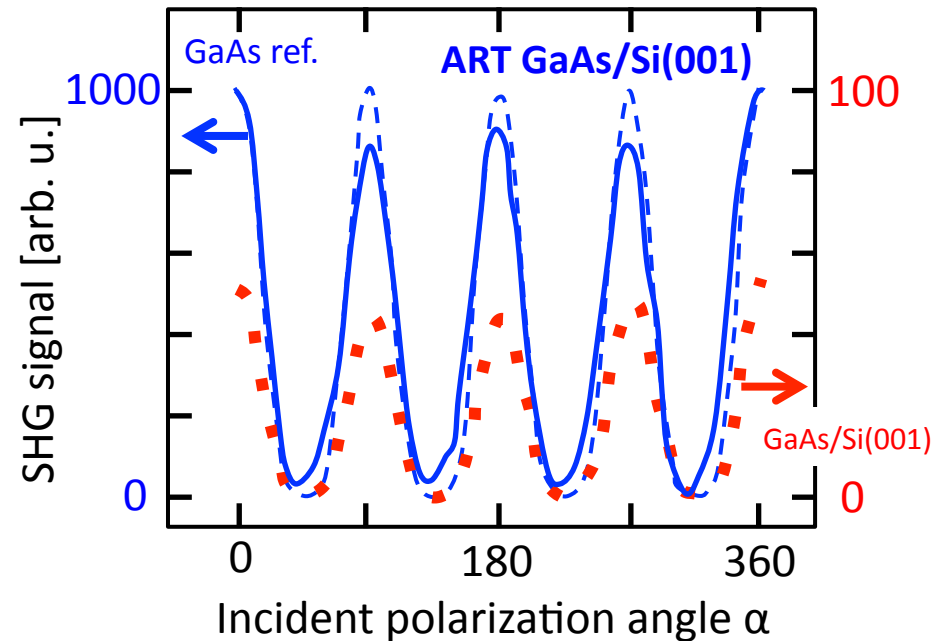
Fitzgerald, *J. Electron. Mater.* **20**, 839 (1991)



3D geometry:



We found (serendipitously) that ART patterning of oriented Si(001) substrates also **dramatically suppresses APDs in GaAs epi-films**



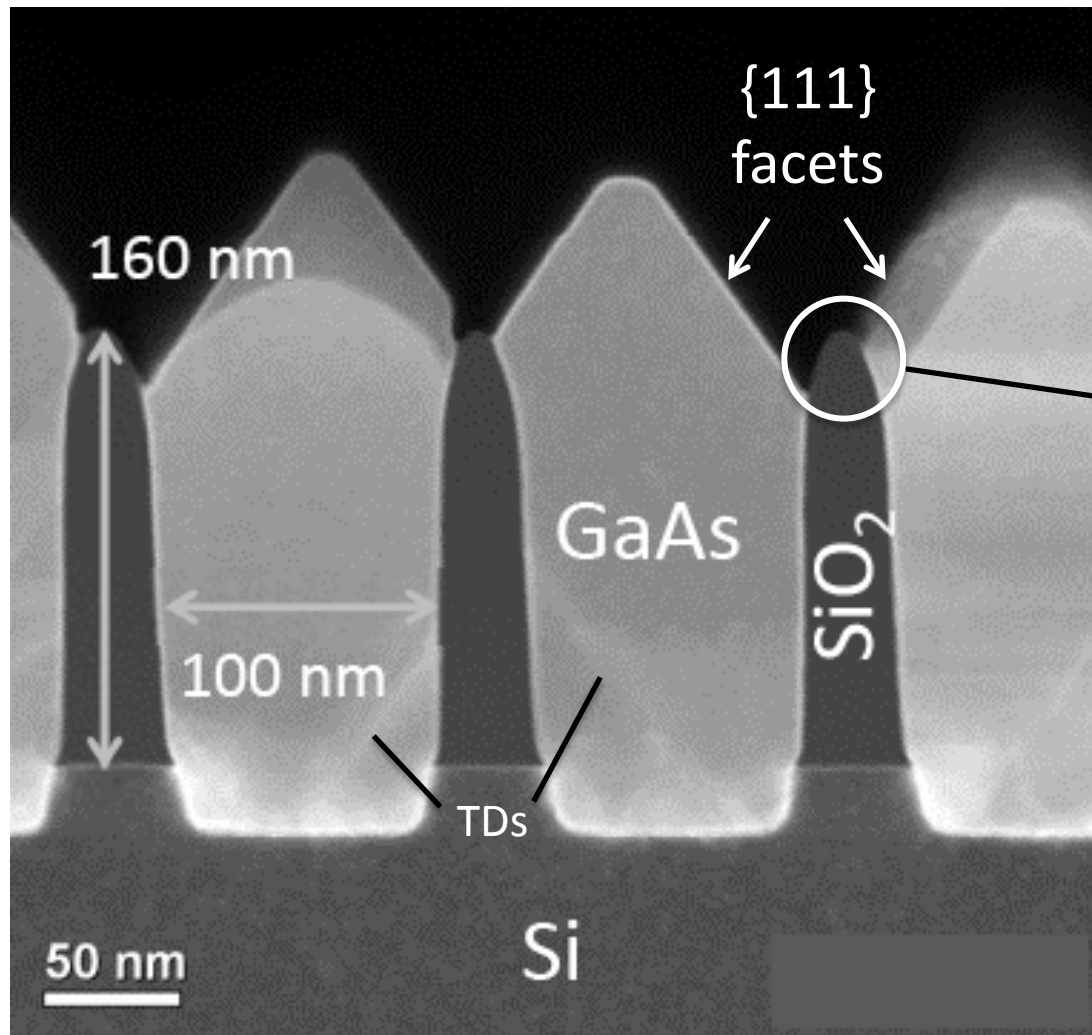
Nearly complete recovery of GaAs reference SHG signal!



GaAs pillars evidently coalesce commensurately into a single domain epi-layer



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tapered sidewall with pliable Si-O bonds may encourage Ga-As bond formation when pillars merge

ART appears to solve 2 problems simultaneously!



SUMMARY



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- SHG characterizes APDs in polar-on-nonpolar semiconductor epilayers sensitively, quickly, non-invasively and selectively.
- Scanning SHG microscopy indirectly probes APD size distribution; SHG-NSOM promises direct APD imaging.
- SHG APD probe helps develop methods to suppress APDs:
e.g. 1. vicinal substrates; 2. ART
- Compared to RAS, SHG is equally useful as an *ex-situ* & *in-situ* APB probe, requires only a single- λ source for any material system, and enables microscopic (possibly single APD) imaging.

Lei et al., Appl. Phys. Lett. **102**, 152103 (2013)
Patent Pending



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