Electronic Localization in Semiconductor Alloys

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Semiconductor alloys

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(InGa)As (InGa)(NAsSb) Ga(AsBi)

EMC-59, South Bend 2017 Characteristics of electronic localization in semiconductor alloys

Low temperature photoluminescence

Fig. 3. Low temperature luminescence spectra of (GaIn)As bulk layers grown by using different As sources as indicated in the inset. The spectrum of the layer grown by using DEtBAs is magnified by a factor of 200.

 $Ga_{1-x}ln_{x}As$ GaN $_{x}As_{1-x}$ GaBi $_{x}As_{1-x}$

011907-3 Kudrawiec *et al.* Appl. Phys. Lett. **94**, 011907 !2009" Appl. Phys. Lett. **94**, 011907 (2009)

σ : intrinsic or extrinsic) Inhomogeneous broadening: intrinsic or extrinsic?

case of DEtBAs non-radiative deep centers, probably

Band structure

Silicon 2-atom basis

Si Silicon 250-atom supercell

Unfolding the first-principle band structure outlined on both patterns is shown on the patterns is shown on the patterns is shown of \mathbb{R} that represents for \mathbb{R} that represents for \mathbb{R} that represents for \mathbb{R} that represents for \mathbb{R} that rep **Unfolding the first-principie**

Plane wave expansion **FRIIC WAVE CAPAIISION**

$$
\Psi_{n,\mathbf{K}}(\mathbf{r})=\sum_{\mathbf{G}}C_{n,\mathbf{K}}(\mathbf{G})\,\mathrm{e}^{i(\mathbf{K}+\mathbf{G})\cdot\mathbf{r}}\qquad\qquad \ldots \atop \ld
$$

D loch a sectuel basis set (such as a Bloch spectral and the Points are expressed in the PW coefficients which was a \sim tions in periodic solids. Here $\frac{1}{2}$ *n* $\frac{1}{2}$ *Cn,*^K(k + g). Thus, the individual "weights" of unfolded *k*weight

$$
w_n(\mathbf{k}) = \sum_{\mathbf{g}} |C_{n,\mathbf{K}}(\mathbf{k} + \mathbf{g})|^2 \qquad \qquad \sum_{\mathbf{\tilde{b}}} 2.0
$$

Popescu & Zunger:
EFECTER for the mapping of the mapp is identical irrespective of whether a supercell or a primitive needs to be generated by translation of the *primitive cell* along Phys. Rev. Lett. **104**, 236403 (2010) 1.0 -cr en
En

a

b

notations in order to distinguish between the reciprocal lattice vectors given the reciprocal lattice vectors given the reciprocal lattice vectors \Box \Box Rubel et al.

of a primitive cell as originally introduced by Popescu and

This generates a multitude of \mathcal{U} unforced of \mathcal{U}

-
-
-

Si $\overline{\mathbf{C}}$

a

with *mⁱ* = 0*,* 1*,...Nⁱ* − 1 that extends up to the scaling fac-

Thermoelectric material: Sio.7Geo.3

In0.53Ga0.47As/InP

1 .
ە 2.5 2.0 1.0 $0.8\big\vert$ Ω 1.5 \circ Spectral Weight Spectral weight Spectral weight $\overline{}$ $\frac{1}{\sqrt{2}}\frac{\sigma}{\sigma}$ Energy (eV) \circ Energy (eV) Energy (eV) 0.6 0.6 1.0 0.5 0.4 0.0 0.0 −0.5 0.2 0.2 -1.0 0^{\perp} 0 \Box G \Box 0 0.5 1 1.5 2 a G $\hbox{\large\it L}$ and $\hbox{\large\it G}$ X and X and X L G X Wave vector Wave vector

> Well preserved Bloch character of the band edges (no localization)

128-atom random alloy models

 $\frac{1}{2}$

 \circ

In0.41Ga0.59N0.03As0.94Sb0.03/GaAs

GaAs0.89Bi0.11/GaAs

Localization of holes is expected

Inverse participation ratio (IPR)

Definition:
$$
IPR(E_i) = \frac{\sum_{\alpha} \rho_{\alpha}^2(E_i)}{\left[\sum_{\alpha} \rho_{\alpha}(E_i)\right]^2}
$$

\nIPR = 1 (extreme localization)

Wegner, Z Physik B **36**, 209 (1980) Murphy *et al*., Phys. Rev. B **83**, 184206 (2011)

(Hg,Cd)Te band structure evolution Hg1−*^x*Cd*x*Te (HCT) is an example of a material system $m \times \alpha$ to GaAs1−*^x*Bi*^x* discussed in the preceding Sec. III B. The Hg1−*x*Cd*x*Te (HCT) is an example of a material system with the topological band inversion [44], which is similar to GaAs1−*x*Bi*^x* discussed in the preceding Sec. III B. The for instance. The electronic structure of GaAs1−*x*Bi*^x* cannot evolve "smoothly" in the range 0 *<x<* 1 and must undergo a topological phase transition. This is a companied with the set of th their symmetry are shown at Fig. 5(a). The conduction band $m \in \mathbb{C}$ volution m for instance. The electronic structure of GaAs1−*x*Bi*^x* cannot evolve "smoothly" in the range 0 *<x<* 1 and must undergo a topological phase transition. This is a companied that the set of the s by a gradual transformation of the host GaAs parabolic their symmetry are shown at Fig. 5(a). The conduction band σ evolution σ and σ

emC-59, South Bend 2017 **Characteristics of electronic localization** in semiconductor alloys ϵ FIG. Couth Rend 2017 He 37, South Bend 2017 (and Hg5Cd22Te27 (b), Hg2Odd3Cd5Te27 (d). The transition of the transition from a seminetary (c), and Hg5Cd22Te27 (a) to an insulator (c), d) or an insulator (c), d) or an insulator (c), d) or an ins S2, South Deng Z017 (and Hg202Te27 (c), Hg1 acter isuts of electronic focanzation in semiconductor ano is an in
Una acter isuts of electronic (c), and insulated (c), d) or an insulator (c), d) or an insulator (c), and insu

Impact of alloying disorder on charge transport a negative band gap to an insulator. The negative gap gradually gap gradually gap gradually gap gradually grad
The negative gap gradually ipact of alloying disorder on char threefold degeneracy is established at a critical composition of the critical composition of the critical compo

 $CdTe \rightarrow (HgCd)Te$ GaAs $\rightarrow Ga(AsBi)$

$$
\mu_{\rm e} = 1,100 \rightarrow 1,000,000 \, \rm cm^2 V^{-1} s^{-1} \qquad \qquad \mu_{\rm e} = 4,000
$$

to GaAs1−*^x*Bi*^x* discussed in the preceding Sec. III B. The

 $\mu_e = 4,000 \rightarrow 2,500 \text{ cm}^2\text{V}$ - s -

Summary

10 • (HgCd)Te

He

- **Ne** • (InGa)As
- Neon 20.1797 • (InGa)(NAsSb) disorder in the conduction band due to electronegative N
- Argon • Ga(AsBi) disorder in the valence band due to electropositive Bi

Further reading: \overline{f}

- Phys. Rev. B **90**, 115202 (2014) **Xe** Xenon
- Phys. Rev. Applied 7, 064011 (2017)
	- Comp. Phys. Commun. **205**, 106 (2016) \bullet
- Phys. Rev. B 93, 205202 (2016)
- $arXiv:1508.03612$ $\overline{2}$
	- arXiv:1707.04625

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图 README.md

Unfolding of first-principle electronic band structure obtained with WIEN2k DFT-(L)APW code

Full potential

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- Anton Bokhanchuk
- Elias Assmann
- Sheikh Jamil Ahmed
- Oleg Rubel

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