Thermodynamic theory of epitaxial alloys: first-principles mixed-basis cluster expansion of (In, Ga)N alloy film

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Thermodynamic theory of epitaxial alloys: first-principles mixed-basis cluster expansion of (In, Ga)N alloy film

Jefferson Zhe Liu and Alex Zunger

± . . //.. Abstract

100 $x = \frac{1}{1} + \frac{1}{1} +$





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Table 1. $\Pi_f(\sigma)$ $\Pi_f(\sigma)$	r	± · /	-	,	777	-
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 $(-m) = \frac{21}{b^{(i)}N^{(i)}} \sum_{b^{(i)} \sigma} \Delta H_{m}(\sigma) \Delta H_{\pm}(\sigma) + .$ $N^{(i)} = \frac{N^{(i)}}{N^{(i)}} \sum_{b^{(i)} \sigma} N^{(i)} = \frac{N^{(i)}}{N^{(i)}} = \frac{N^{$ C,

Table 2. ±	-	- , r	/ 	°00 r		, L , I	bulk ¹		c.
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		<u>, , , , , , , , , , , , , , , , , </u>	с. Т. с. с.		71	1 1/ * 1 */	· / I .		
$(\)_{i} (\)$	β,,,-,, ±,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	γ., γ.,		α,, μ	<u>*</u> 4	/ 11 / 17) / 12	/ *	, ī	±,,, *, , ,, -,
$()_{i} ()_{i} ()_{i}$	β, η ¹ β, η ¹ α ⁴	7ι Υ, Α	<i>ī</i> ,	α,	1 2	¥ (4`]) 4 : 4 4	4 . 4 <u>*</u>		. 4
(), ()	, , , , , , , , , , , , , , , , , , ,	, , -	·	· · · · •] *	- 71				± (▲ ↘ ₹▲
				ſ		$\Delta H_{\!_{\pm}}$	(σ)	$\Delta H_{-}(\sigma)$, r	
L		V,	/	r – – L	L		<u>+</u>	r _	
·	r	Ĩ	L		2.3. Calci	ulation of 2	$\Delta H_{LDA}^{epi}(\sigma)$ ΔH_{\pm}) (σ)	1
		-	r _			,	<i>,</i> ±	× × =	
				<i>m</i> ⁻					
-	L	,	_						
, $\Delta_{\sigma}^{(m)} > 1$,	, > <u>,</u> / L	717	-,1	L _					
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L -	<i>'oo</i> '								
,	,' L	1	L						

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Figure 6.

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Figure 11.
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5. Summary



100 -TTr **4** L --

$$\int \Delta H_{\pm} (\sigma) -$$

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- - **21**

