

Relativity-Induced Ordering and Phase Separation in Intermetallic Compounds

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Relativity-Induced Ordering and Phase Separation in Intermetallic Compounds.

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First, deform hydrostatically pure A and B from their equilibrium volumes V_A and V_B to the volume V akin to the final compound σ with composition x . In doing so we invest a

Since the input to eq. (6) is a set $\{A, U, \dots\}$ of formation potentials for ordered compounds

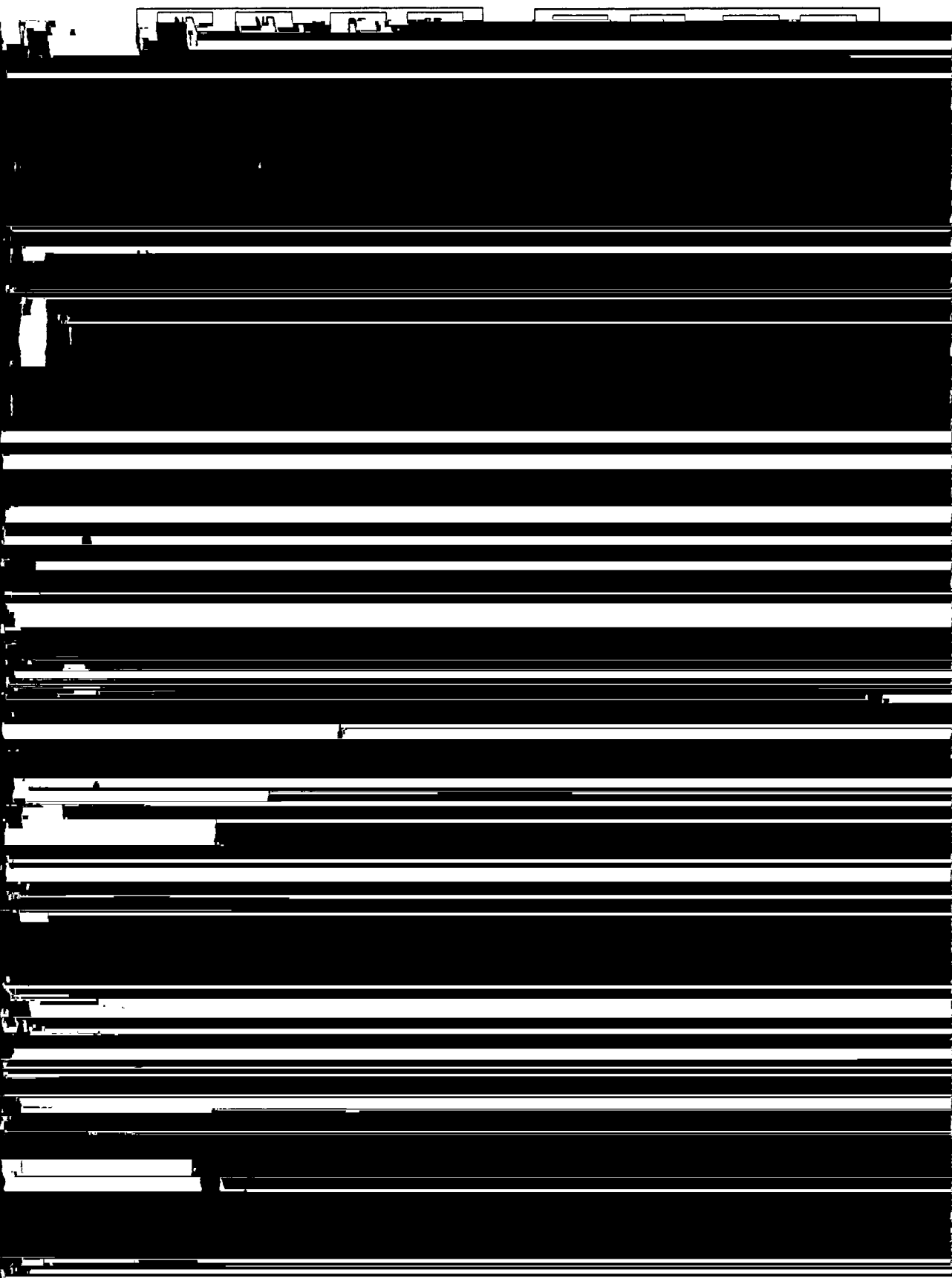


TABLE I. - Contributions of volume deformation (VD), charge exchange (CE), and relaxation (REL) to

	Nonrelativistic		Relativistic	
	Γ_1	Random	Γ_1	Random
Ni_{0.5}Pt_{0.5}				
ΔE_{VD}	+ 543.6	+ 543.6	+ 426.8	+ 426.8
ΔE_{CE}	- 398.4	- 307.0	- 504.5	- 403.3
ΔE_{REL}	- 51.6	- 60.5	- 18.0	- 53.8
ΔH	+ 93.6	+ 176.1	- 95.7	- 30.3
δE_{ord}	- 82.5	—	- 65.4	—
Au_{0.5}Pt_{0.5}				
ΔE_{VD}	+ 42.3	+ 42.3	+ 48.6	+ 48.6
ΔE_{CE}	- 113.5	- 103.5	+ 28.2	+ 1.5
ΔE_{REL}	~ 0	~ 0	~ 0	~ 0
ΔH	- 71.2	- 61.2	+ 76.8	+ 50.1
δE_{ord}	- 10.0	—	+ 26.7	—
Ni_{0.5}Au_{0.5}				
ΔE_{VD}	+ 722.2	+ 722.2	+ 561.8	+ 561.8
ΔE_{CE}	- 337.8	- 283.8	- 464.8	- 369.2
ΔE_{REL}	- 11.9	- 82.5	- 20.2	- 68.3
ΔH	+ 372.5	+ 355.9	+ 76.8	+ 124.3
δE_{ord}	+ 16.6	—	- 47.5	—

