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VIBRATIONAL MECHANICAL AND THERMAL PROPERTIES OF III-V
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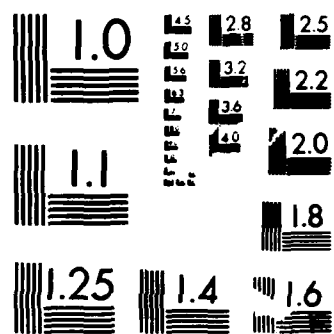
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DATE: 29 September 1987

FOR THE PERIOD: 1 September 1986 to 31 August 1987

AFOSR Contract No: AFOSR-85-0331

TITLE: Vibrational, mechanical, and thermal properties of III-V semiconductors

PRINCIPAL INVESTIGATOR: John D. Dow

1. SUMMARY

Theories of the mechanical, vibrational, and electronic properties of III-V semiconductors have been developed and applied to (i) help determine the feasibility of InN-based visible and ultraviolet lasers and light detectors, (ii) develop a theory of phonons in semiconductive alloys, (iii) elaborate on the physics of photoelasticity, (iv) understand surface reconstruction of semiconductors, and (v) predict the effects of atomic correlations on the light-scattering (Raman) properties of semiconductive alloys.

2. OBJECTIVES

Our goal is to develop theories of the mechanical, vibrational, and thermal properties of III-V semiconductor alloys that will lead to a better understanding of the physics of these materials.

3. STATUS OF RESEARCH

We have made progress on the following problems:

1. Electronic structure of InN and InN-based alloys, including defect levels. A paper will be published shortly on the materials problems that must be overcome in order to fabricate visible lasers from these materials.
2. Phonons in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$. We have identified the "clustering modes" with regions consisting of Te atoms bonded to one Cd atom and three Hg atoms; and we have elucidated the physics of phonons in these alloys.
3. Photoelastic constants. We are developing a theory of photoelastic constants in bulk and superlattice semiconductors.
4. Role of ionicity in zincblende surface relaxation. We have shown that, contrary to popular opinion, zincblende (110) surfaces relax through an angle that depends significantly on ionicity, as a result of competition between covalent forces seeking 90° bond-angles and ionic forces that resist reconstruction.
5. Surface geometry of wurtzite (1010) surfaces. We are calculating the equilibrium positions of atoms on (1010) surfaces of AlN and ZnS.
6. Effects of correlations on the Raman spectra of alloys. We have developed a theory which combines Monte Carlo and Recursion techniques to predict the spectra of correlated alloys.

4. RECENT PAPERS

1. S. Lee and J. D. Dow. Electronic structure of $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$ semiconductor alloys. Phys. Rev. B in press.
2. R. V. Kasowski, M.-H. Tsai, and J. D. Dow. Dependence on ionicity of the (110) surface relaxations of zincblende semiconductors. J. Vac. Sci. Technol. submitted.
3. Z.-W. Fu and J. D. Dow. "Clustering modes" in the vibrational spectra of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ alloys. Phys. Rev. B in press.
4. M.-H. Tsai, R. V. Kasowski, and J. D. Dow. Relaxation of the non-polar (10 $\bar{1}$ 0) surface of wurtzite AlN and ZnS. Solid State Commun. 64, 231-3 (1987).
5. A. C. Redfield and J. D. Dow. Theory of Raman spectra of correlated substitutional alloys. Solid State Commun. in press.
6. D. W. Jenkins and J. D. Dow. Electronic structures and doping of InN, $\text{In}_{1-x}\text{Ga}_x\text{N}$, and $\text{In}_{1-x}\text{Al}_x\text{N}$. Ph.D. thesis chapter completed; manuscript in preparation.
7. M.-H. Tsai, R. V. Kasowski, and J. D. Dow. Relaxation of zincblende (110) surfaces. manuscript in preparation.
8. Z.-W. Fu and J. D. Dow. Phonons in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$. manuscript in preparation.

5. PROFESSIONAL PERSONNEL

J. Dow, principal investigator
S. Ren, visiting professor
W. Hu, visiting associate professor
M. Tsai, assistant faculty fellow
D. Jenkins, graduate student
R. Hong, graduate student
J. Shen, graduate student
Z. Fu, graduate student

6. INTERACTIONS

The principal investigator has functioned as an advisor to the National Academy of Science Committee on Basic Research on a wide range of topics in materials science, electronics, and solid state physics, and to the Air Force (Capt. K. Malloy) on matters related to semiconductor alloys.

PATENTS

None.

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Dependence on ionicity of the (110) surface relaxation
of zincblende semiconductors

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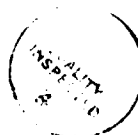
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Abstract

It is argued that the surface relaxation angle ω of zincblende (110) surfaces should depend on ionicity or on longitudinal effective charge Z , approximately as $\omega = \omega_0 - \omega_1 Z^2 e^2 / \epsilon a_L$, with $\omega_1 = 6^\circ/\text{eV}$.

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It is widely believed that the reconstructions of the (110) surfaces of zincblende semiconductors are determined virtually exclusively by covalent forces, and that the surface anions rotate more-or-less rigidly out of the surface through an angle $\omega \approx 29^\circ$ for all zincblende (110) surfaces [1][2]. (See Fig. 1.) This relaxation angle ω minimizes the energy of the covalent bonds. Indeed the (110) zincblende relaxations are thought to be the best understood of the semiconductor surface reconstructions, with analyses of numerous low-energy electron-diffraction data [1][3][4][5][6][7] and medium-energy ion-blocking experiments [8][9][10] lending support both to the rigid-rotation reconstruction model and to the notion that ω is constant ($\approx 29^\circ$) for all zincblende (110) surfaces.

However, the widely accepted viewpoint that ω is constant for all zincblendes cannot possibly be correct, and must be strictly valid only in the limit of low ionicity. For the more ionic zincblende semiconductors, the attractive Coulomb forces between the relaxed, negatively charged surface anions and the positively charged cations in and below the surface tend to pull the anions back toward the surface and reduce the relaxation caused by the covalent forces. (See Fig. 1.) This Coulombic effect should reduce the relaxation angle ω by an amount proportional to Z^2 , where Z is the (longitudinal) effective charge [11], and the effect should become significant when $Z^2 e^2 / \epsilon a_L$ is of order 0.5 eV, a typical covalent energy gained by each relaxing surface anion [12]. Here e is the electron's charge, ϵ is the dielectric constant, and a_L is the lattice constant. Recall that the ionicity f_i is approximately proportional to Z : $Z/Z_C \approx f_i$, where Z_C is the chemical valency [11].

To demonstrate that the relaxation angle ω cannot be the same for all zincblende semiconductors, we have executed self-consistent total-energy calculations based on the pseudo-function local-density theory [13]. These calculations employed four-atom-thick slabs of GaAs, InP, ZnTe, and ZnS [14], and allowed their (110) surfaces to relax via rigid rotations through angles ω until the total energies of the slabs reached minima. The resulting equilibrium relaxation angles ω are plotted in Fig. 2 as functions of $Z^2e^2/\epsilon a_L$ (See Table I.), and, to a good approximation, form a straight line described by the empirical rule

$$\omega = \omega_0 - \omega_1 Z^2e^2/\epsilon a_L,$$

with $\omega_0 = 20.62^\circ$ and $\omega_1 = 6.08^\circ/\text{eV}$. The fact that ω_0 is of the same general magnitude as the observed surface relaxation angles indicates that the rigid rotation model, as used here, contains the essential physics of the surface relaxation. Furthermore, the sign and magnitude of ω_1 are as expected.

The relaxation angles ω extracted from data analyses are difficult to obtain accurately (See Table I.), and actually agree about equally well with either hypothesis; (1) the widely believed $\omega = \text{constant}$ or (2) $\omega = \omega_0 - \omega_1 Z^2e^2/\epsilon a_L$, with ω_1 of order $6^\circ/\text{eV}$. (See Fig. 2.) Therefore we think that the $\omega = \text{constant}$ hypothesis should be reexamined experimentally, possibly by studying the (110) surface of zincblende AgI or some other highly ionic zincblende material.

The ionicity of the zincblende surface not only reduces the equilibrium relaxation angle ω , but it also increases the relaxation energy per surface atom and increases surface phonon frequencies, according to the theory. (See Fig. 3.)

We hope that experiments on the (110) surfaces of different zincblende semiconductors will confirm these theoretical ideas quantitatively, establish the role of effective charge and ionicity in determining equilibrium surface geometry, and lead to an even better understanding of these prototypical surfaces.

Acknowledgments -- We gratefully acknowledge enlightening conversations with Richard Martin about effective charges, and the support of the Air Force Office of Scientific Research (Contract No. AF-ASFOSR-85-0331). We also thank the E. I. du Pont Company for the use of their computational facilities, as well as partial support of M.-H. Tsai.

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- [14] The calculations for each material require about 150 hours of central processor time on an FPS-164 array processor.

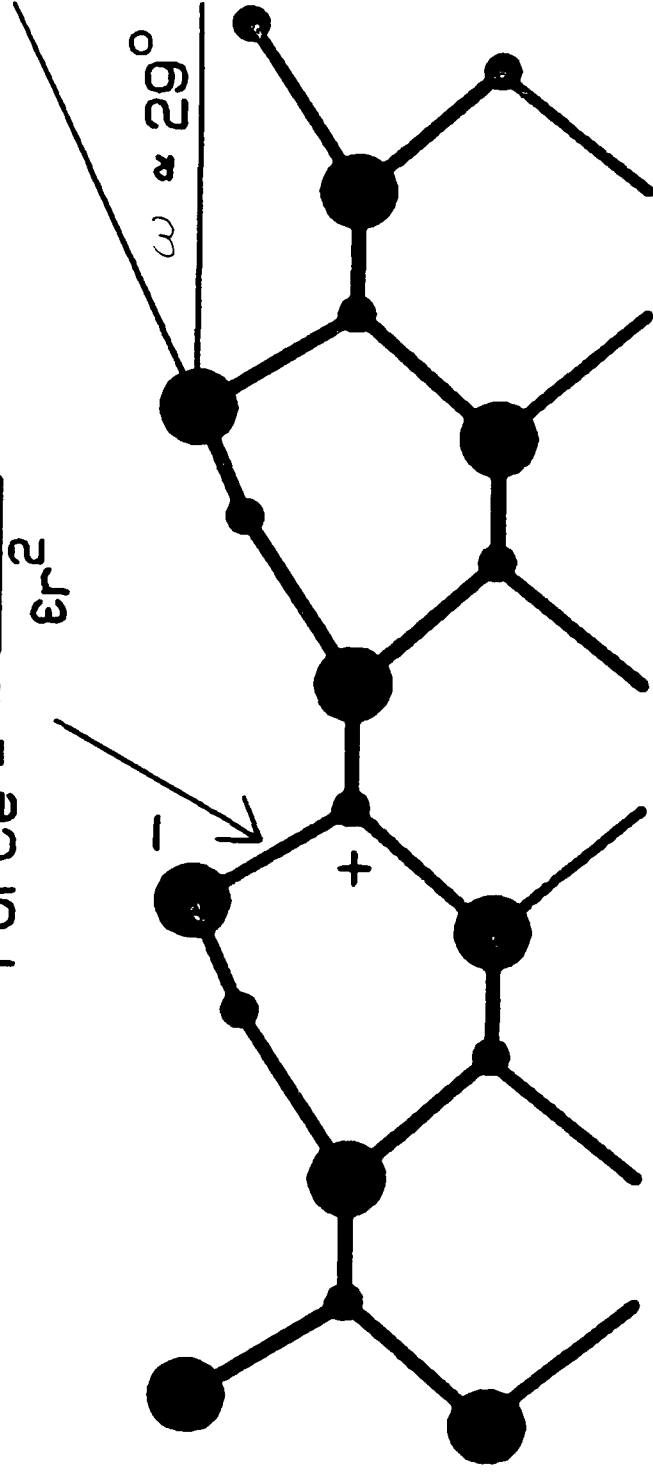
Table I. Effective (longitudinal) charges Z , lattice constants a_L (in unit of Bohr radii), dielectric constants ϵ , $Z^2 e^2 / \epsilon a_L$ (in eV), calculated relaxation angle ω_{Theory} , predicted change in relaxation angle $\Delta\omega$ (based on the empirical rule), and relaxation angles ω measured by low energy electron diffraction (ω_{LEED}) and ion back-scattering (ω_{ion}), respectively. See Ref. [11].

Materials	Z	$a_L(a_0)$	ϵ	$Z^2 e^2 / \epsilon a_L$	ω_{Theory}	$-\Delta\omega$	ω_{LEED}	ω_{ion}
CuCl	1.505	10.215	3.6	1.67		10.15°		
CuBr	1.35	10.753	4.4	1.048		6.37°		
CuI	1.715	11.419	5.2	1.347		8.19°		
AgI	1.38	12.232	4.9	0.864		5.25°		
ZnS	1.795	10.222	5.1	1.681	11°	10.22°	26° [3]	
ZnSe	1.625	10.710	5.9	1.137		6.91°	29° [4]	
ZnTe	1.66	11.529	7.3	0.891	14°	5.42°	28°±2° [5]	
CdTe	1.715	12.240	7.3	0.895		5.44°		
HgTe	2.025	12.208	14.0	0.653		3.97°		
BN	0.78*	6.831	4.5	0.538		3.27°		
AlP	0.93*	10.301	7.6	0.301		1.83°	27.5°±3° [6]	
AlAs	0.81*	10.700	9.0	0.185		1.12°		
AlSb	1.045	11.594	10.2	0.251		1.53°		
GaP	1.185	10.300	8.5	0.436		2.65°	27.5° [3]	
GaAs	1.03	10.683	10.9	0.248	20°	1.51°	27°-31° [3]	29°±3° [9]
GaSb	0.69	11.519	14.4	0.078		0.47°	30°±2° [5]	28.5°±2.6° [10]
InP	1.485	11.090	9.6	0.563	17°	3.42°	28.1° [8]	
InAs	1.085	11.449	12.3	0.227		1.38°	31°±3° [7]	30°±2.4° [10]
InSb	0.72	12.243	15.6	0.074		0.45°	28.8° [8]	
SiC	0.775	8.217	6.7	0.297		1.81°		

* Estimated from the ionicity f_i by $Z = Z_c f_i$.

Zincblende (110) surface side view

$$\text{Force} \propto -\frac{Z^2 e^2}{\epsilon r^2}$$



Coulomb force pulls surface anions down

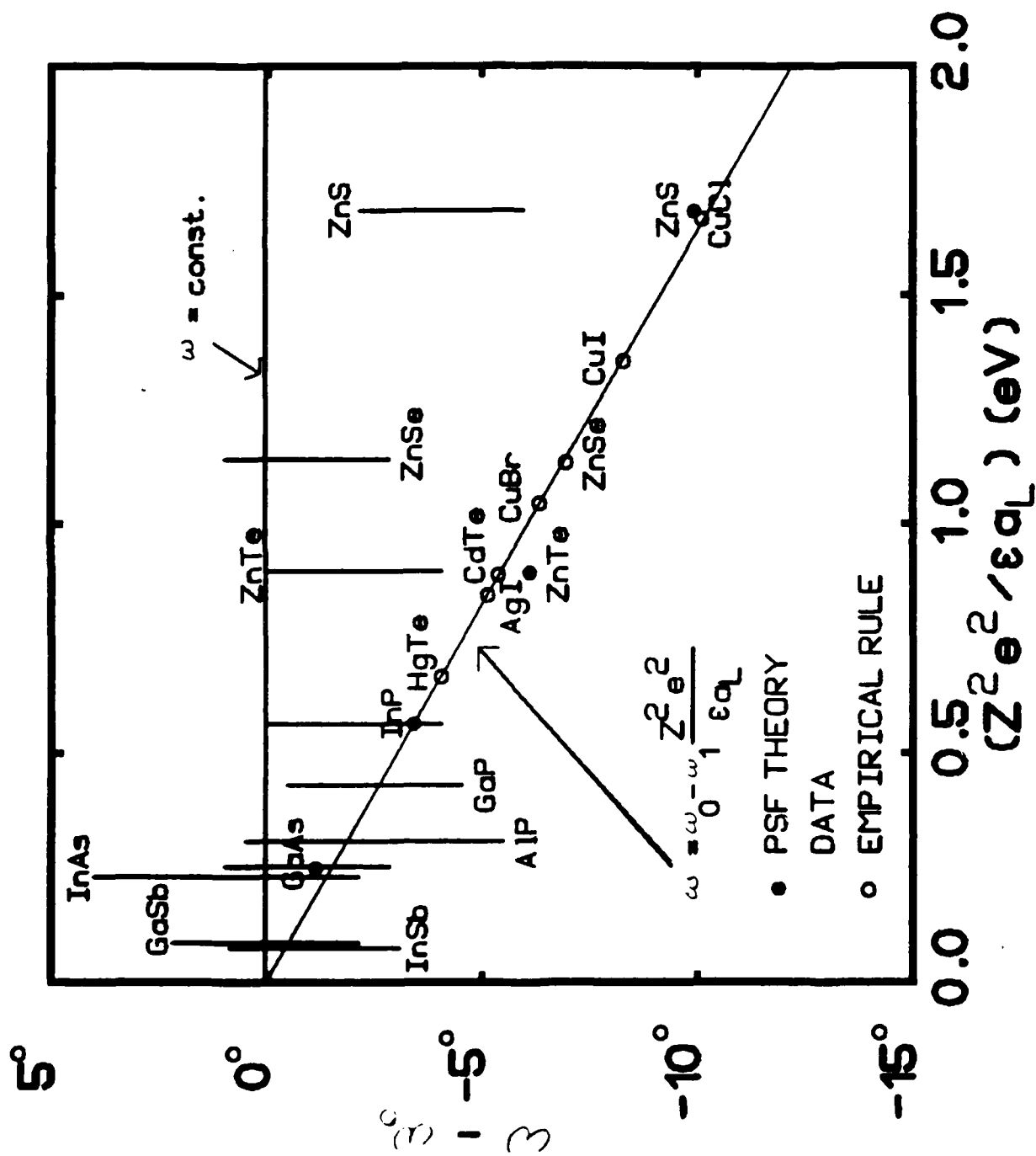


Fig. 2

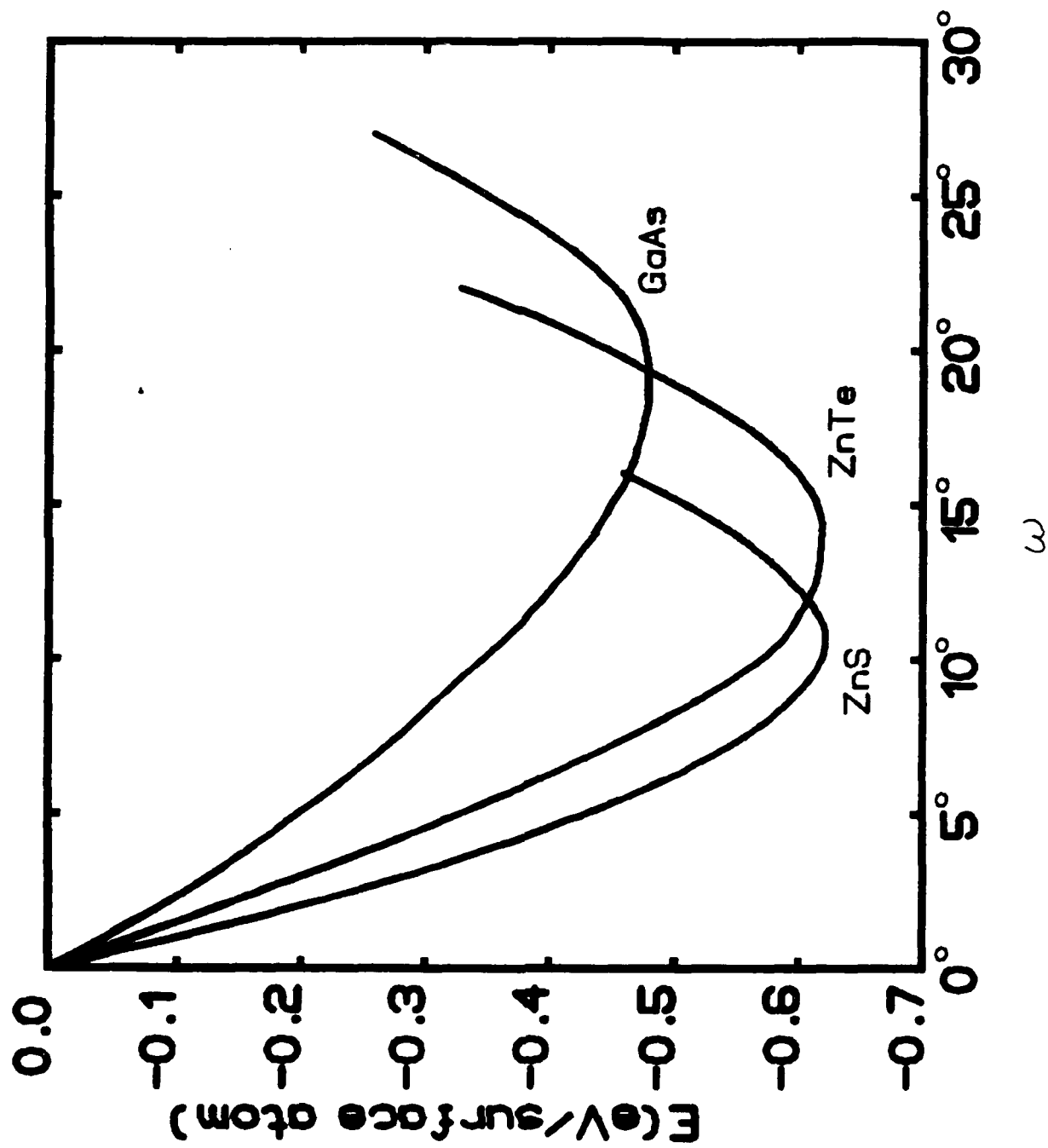


Fig. 3

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