

苟清泉论文选集(续集)

The Sequel to Selected Works of
Gou Qingquan

《苟清泉论文选集(续集)》编委会 编

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内 容 简 介

苟清泉教授从事科教工作近七十年,为了祝贺他的重大成就与贡献,特编辑此论文选集。本文集(续集)主要收录其1991年以后发表的论文57篇,内容涵盖了原子分子物理、固体物理、高压物理及高压合成等领域。通过这些论文可以较全面地了解他20世纪90年代至今在原子分子物理、固体物理及高压科学等领域的学术成就。本文集反映了苟清泉教授探索、创新、奉献的科学精神,与1992年出版的《苟清泉论文选集》共同见证作者的科学人生。

本文集可供高等院校和科研院所原子分子物理、固体物理、高压物理和高压合成的相关专业人员参考,也可作为相关专业师生的教材。

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序 言

苟清泉教授于1917年4月14日出生于四川省邛崃县,1942年毕业于国立中央大学物理系。大学毕业后,他先后在国立中央大学、西南联大、北京大学、华西大学、南京大学、四川大学、东北工学院、吉林大学和成都科技大学从事教学与科研工作,已达六十五年之久。

他长期从事原子分子物理、固体物理、高压物理及高压合成等方面的科研与人才培养工作,取得了系统的、创造性的科技成就,作出了重大贡献,培养了大量的优秀人才,是我国原子与分子物理学科的创始人及高压物理与合成研究的奠基人之一。他先后创建了中国科学院东北物理所、吉林大学原子与分子物理研究所及成都科技大学高温高压与原子分子科学研究所,均为首任所长。这些都为我国的原子分子物理及高压物理与合成领域的发展起到了重要的学术带头和推动作用。他从1962年起被聘为国家科委物理学科组和冶金组成员,参与制订了国家科学发展规划,兼任中国科学院东北分院院务委员。从1955年起任中国科学院金属研究所学术委员。曾长期担任中国物理学会及中国力学学会的理事,兼任中国物理学会原子与分子物理专业委员会主任及中国力学学会物理力学专业委员会主任,并兼任过四川物理学会理事长。从1984年起任《中国科学》编委及《原子与分子物理学报》主编,从1987年起任《高压物理学报》主编,从1985年起任国际重要刊物《Journal of Physics and Chemistry of Solids》顾问编委。1986年曾任意大利国际理论物理中心暑期讨论班高压物理组的研究领导人。1985~1986年曾被聘为美国克里斯坦森超硬材料研究中心顾问。1990年以后曾三次应邀到日本筑波大学材料研究所和日本科技厅无机材料研究所讲学。现为四川大学原子分子物理博士点重点学科的学术负责人,高温高压与原子分子科学研究所的名誉所长,兼联合所(与中国工程物理研究院一所联合建立的高温高压物理所)的名誉所长,负责学科建设与博士生的培养工作。另外,他还是上海交通大学和西安交通大学的兼职教授。

苟清泉教授长期从事原子解析波函数的系统研究,已将发表的一系列论文整理总结写成了专著《原子结构的变分计算》,获得了国家教委的优秀专著奖。在慢电子与原子分子碰撞方面,他提出了物理模型与计算方法,取得了大量的科研成果。近年来,他在对氢原子集团的研究方面取得若干新结果,得出了“高压合成金属氢是可能的”这一重要结论。他从原子分子物理出发,对人造金刚石的高压合成机理进行了深入研究,提出了自己的创造性理论,写出了专著《人造金刚石合成机理研究》,对指导人造金刚石的合成研究与生产起到了很大的推动作用,为我国人造金刚石的发展作出了重大贡献。其深厚造诣,已使他成为人造金刚石合成这个重要领域里国际著名的学者。

早在1989年,苟清泉教授首先从原子分子及晶体物理出发进行分析研究,提出一种理论阐明在晶体中常温核聚变是可能实现的,并预言这种聚变反应以放热为主,同时放出 ^4He ,放出的中子与质子比较小。此预言为当年由他组织的、朱正和与张清福两位教授领导的实验研究所证实,后来为世界各国很多单位所验证。在他的带动下,促进了国内这方面研究的开展。早在十年前,他带头承担了国家“863”高技术科研课题“新材料的原子分子设计”,提出了许多新思想新观点,取得了显著成绩。近三年来,他提出了从原子间相互作用出发建立高温超导新理论及强相互作用与库仑相互作用的统一理论,学术思想一直很活跃。

苟清泉教授十分重视和提倡理工结合,提倡自主创新,发展新科学技术。早在1984年,在成都科技大学创建高温高压物理研究所(后改名为高温高压与原子分子科学研究所)的同时,在两弹元勋邓稼先院士的支持下,他积极与中国工程物理院一所在校内联合创建了“应用物理研究所”,由他与中物院科技委副主任经福谦院士任所长。稍后,在钱学森院士的建议下,他支持朱正和教授积极与中物院二所在校内联合创建了“原子与分子工程研究所”,由朱正和教授与中物院科技委副主任傅依备任所长。三个所的建立,形成了三位一体的联合体,侧重研究高温高压下的原子分子状态、相互作用及新材料的原子分子设计与高温高压合成。他得到的经验是:发展学科必须走联合发展的道路。四川联合大学成立后,他进一步努力吸引校内相关学科参加协作,扩大合作范围,形成“原子分子科学与工程中心”。他同时还与29基地建立科研合作组,由他与乐嘉陵院士任组长,并与核工业西南物理研究院加强联系同时兼任该院的科技顾问,主持了中国环流器新一号装置的验收鉴定工作。经过他的努力,学校与国家在四川建立的几个大科研基地先后建立了密切的联系与合作关系。

在学科建设中,他为原子分子物理和高压物理学科制订了正确的发展方向,发展了与国际间的科研合作与交流。他与日本高柳和夫教授共同发起中日原子分子物理学术讨论会,现已发展成为亚洲国际原子分子物理讨论会;他创办的《原子与分子物理学报》和《高压物理学报》两种中国核心期刊,成为青年科技工作者的学术园地,使学科建设不断向前发展,欣欣向荣,优势突出。

苟清泉教授从事科教工作五十五周年时,为了庆祝他的卓越贡献,中国物理学会原子与分子物理专业委员会、中国力学学会物理力学专业委员会和四川物理学会在他八十华诞之际联合在四川联合大学召开学术会议,总结他的学术思想,进行学术交流。会议上报告的论文大部分发表在《原子与分子物理学报》的专刊中。在他九十华诞之际,我们带着兴奋的心情,庆祝苟清泉教授从事科教工作六十五周年,举行学术讨论会,出版专刊,以庆祝他为我国的科教事业和人才培养作出的重要贡献。我们要在苟清泉教授的学术思想指导下,为发展我国原子分子物理、固体物理、高压物理及高压合成等科学而努力奋斗,不断取得新成绩。

1992年,为了祝贺苟清泉教授从事科教工作五十年,我们编辑了《苟清泉论文选集》,

由科学出版社出版。2007年是苟清泉教授从事科教工作六十五周年,为了祝贺他的重大成就与贡献,我们编辑了这本论文续集,主要收集他1991年以后发表的论文,仍由科学出版社出版。我深信这两本论文选集不仅是我国原子分子物理、高压物理与合成科研方面发展历程中许多重要里程碑的历史记录,而且是两本自成系统的科学著作。

朱正和

2007年10月30日于四川大学

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第一篇

高压固体状态方程

THEORETICAL CALCULATION FOR THE EQUATION OF STATE AND PHASE TRANSITION OF LITHIUM HYDRIDE CRYSTAL

QINGQUAN GOU, XINQIANG WANG and JINFANG MENG

Institute of High-Temperature and High-Pressure Physics, Chengdu University of Science and Technology, Sichuan, P.R. China

(Received June 21, 1989)

From the point of view of overlapping interactions between the nearest neighbours, while considering the compression effect of each ion, an ionic overlap-compression model is founded and applied to lithium hydride. The repulsive potential and cohesive energy curves of the crystal are calculated by a one-parameter variational method. The obtained equilibrium lattice constant ($3.865 a_0$), cohesive energy (-218.82 kcal/mol), and bulk modulus (353 kbar) agree with experimental values surprisingly well. The calculated values of the equation of state also reach a good agreement with the experimental ones available below 40 kbar. A phase transition from NaCl to CsCl structure is predicted to occur around 0.85 Mbar, with a volume jump of about 6%.

KEY WORDS: Ionic overlap-compression model, equation of state, phase transition, lithium hydride.

1 INTRODUCTION

Lithium hydride (LiH) is an important material, and also the simplest one in ionic crystals. The first quantum mechanical investigation about it was carried out by Hylleraas¹ in 1930, where the Heitler-London scheme was applied to a solid-state problem. After that, the same approach was used by other authors², though Lundqvist³ had pointed out that Hylleraas' results only corresponded to the first order in a highly divergent expansion of overlap integrals of the wave functions centered on various ions. Ewing and Seitz⁴ firstly used the cellular method of band theory to calculate the single-electron band structure of LiH crystal. A relatively new calculation for its band structure was made by Kunz and Mickish⁵.

The theoretical studies mentioned above did not deal with the equation of state and phase transition. But now, much attention is paid to the high pressure properties of LiH crystal because of its important use in nuclear fusion researches. The problem of phase transition is the focus to study all the time. Schumacher⁹ firstly used the semiempirical Born-Mayer method to estimate that a NaCl-to-CsCl structure transition in LiH crystal would occur at about 4 kbar. But subsequent experimental studies did not find such a transition up to 0.5 Mbar¹⁰⁻¹². On the other hand, there have been a few theoretical studies for its high pressure properties by using the methods of band theory. Among them may be mentioned the works of Perrot¹³ and Hama *et al.*¹⁶, where the equation of state and the

metallization of LiH crystal under high pressure were studied, but the transformation from NaCl to CsCl structure was not concerned. From another aspect, Hammerberg¹⁴ predicted that the first metallization of LiH crystal will occur at about 2 Mbar, while its structure will change from NaCl to CsCl type. Whether such a structural phase transition exists or not still needs, however, to be confirmed by high pressure experiments above 0.5 Mbar. And a further theoretical study of this problem is also very useful.

In this paper, we propose a new theoretical model, in which the compression effect of ions in the crystal is considered. A detail description of this model will be given in the following part. All the results will be presented in the later part.

2 THEORETICAL MODEL

2.1 *Basic Idea*

Generally, every ion in an ionic crystal has a closed shell structure similar to a noble gas atom, and the interactions of each ion with all the others possess a rather high degree of symmetry, especially for NaCl and CsCl structures. If we approximately take such a symmetry as a spherical type, then the wave function of each ion in the crystal will keep its spherical symmetry unchanged as an isolated one. Therefore, when we calculate the repulsive interaction between such two ions, the effects of all the neighbours can be considered naturally. From this point, we may simplify a many-body problem in an ionic crystal to a two-body one. Furthermore, we find that the compression effect of ions must be taken into account, especially in alkali hydride crystals under high pressure. At the same time, we noticed the work of Fischer *et al.*¹⁵, in which the repulsive potential of LiH crystal was calculated under two-body approximation by Heitler-London method, but the compression effect was not included. So their results were not good compared with the experiment. Actually, because the distribution of the two electrons around the nucleus of a H^- ion in alkali hydrides is rather loose, it is easy to be compressed. This effect gives a large modification to the repulsive interaction. It is unreasonable to ignore this fact. We should emphasize that overlap and compression effects are two inseparable aspects of the interactions between ions in an ionic crystal under high pressure. This is just the key point to establish our new model.

2.2 *Ionic Overlap-Compression Model*

This model is based on the following two assumptions:

- i) The wave function of each ion in the crystal overlaps only with the nearest neighbours.
- ii) The wave function of each ion keeps its spherical symmetry unchanged during compression.

A schematic description of the model is shown in Figure 1. Let $\psi_{\pm}^{(i)}$ ($i=1, 2, 3$) be the wave functions of a positive ion or a negative one in three different states with energies $E_{\pm}^{(i)}$, respectively.

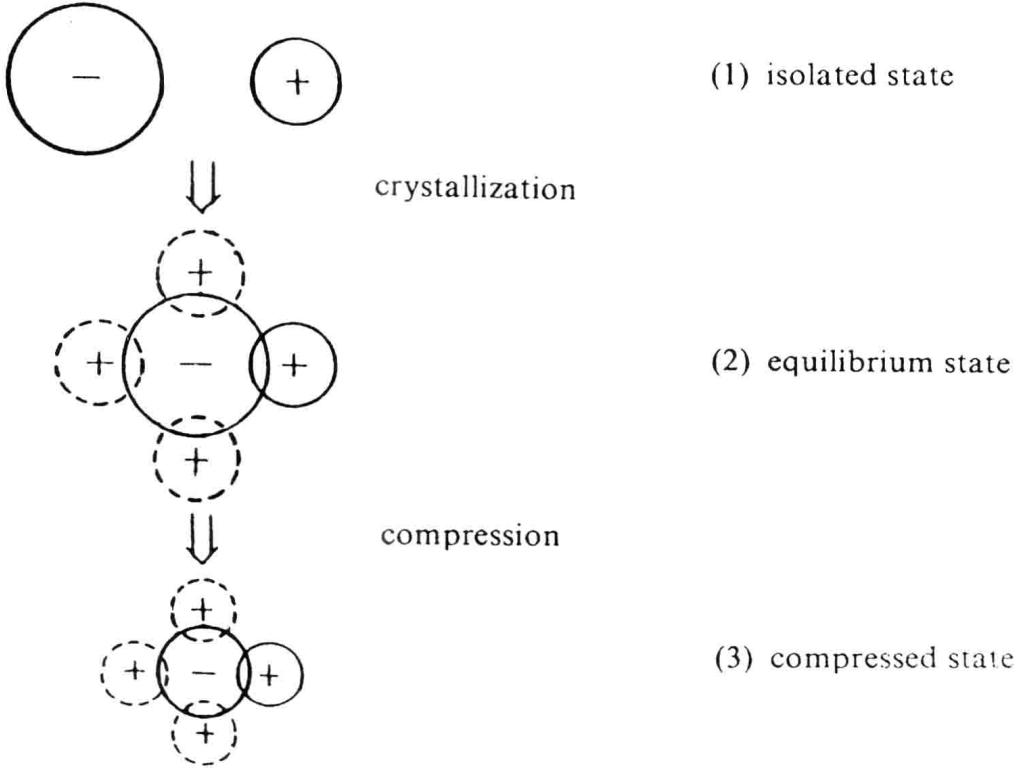


Figure 1 Ionic overlap-compression model.

In two-body approximation, the repulsive overlapping interaction between a positive ion and a negative ion is defined as

$$V_{ol}^{+-}(R) = \frac{\langle \Psi^{(i)} | \hat{H} | \Psi^{(i)} \rangle}{\langle \Psi^{(i)} | \Psi^{(i)} \rangle} - (E_+^{(i)} + E_-^{(i)}) + \frac{2Z_+ Z_-}{R}, \quad (1)$$

where \hat{H} is the total Hamiltonian of the two-ion system, $\Psi^{(i)} = \hat{A}(\psi_+^{(i)} \psi_-^{(i)})$ the total antisymmetrized wave function (\hat{A} the antisymmetrization operator), Z_{\pm} the number of the net charge of a positive or a negative ion ($Z_{\pm} = 1$ for LiH), and R the interionic distance. All the expressions in this paper are in Rydberg atomic unit. The energy change of a "single" ion because of compression is defined as

$$\Delta E_{\pm} = E_{\pm}^{(i)} - E_{\pm}^{(1)}. \quad (2)$$

According to assumption (i) and above two definitions, we can deduce the expression of the cohesive energy as following.

If there are N pairs of ions in the crystal, the total cohesive energy is

$$U = \frac{1}{2} \sum_{i \neq j}^{2N} V_{ij} \quad (3)$$

where V_{ij} is the interaction potential between i and j ions. If we neglect the surface effect, all the positive (or negative) ions can be treated as equal. Then we have

$$U = \frac{1}{2} N \left(\sum_{j \neq 1}^{2N} V_{1j}^+ + \sum_{j \neq 2}^{2N} V_{2j}^- \right), \quad (4)$$

where

$$\sum_{j \neq 1}^{2N} V_{1j}^+ \left(\sum_{j \neq 2}^{2N} V_{2j}^- \right)$$

is the sum of the interactions of a positive (negative) ion with all the others. In present model, the sum includes three parts: (i) Coulomb potential (or Madelung term), (ii) repulsive overlapping interaction potential, and (iii) the energy change of the ion because of compression. So we have

$$\sum_{j \neq 1}^{2N} V_{1j}^+ = -\frac{2\alpha_m Z_+ Z_-}{R} + M \cdot V_{ol}^{+-}(R) + \Delta E_+ \quad (5)$$

and

$$\sum_{j \neq 2}^{2N} V_{2j}^- = -\frac{2\alpha_m Z_+ Z_-}{R} + M \cdot V_{ol}^{+-}(R) + \Delta E_- \quad (6)$$

where α_m is the Madelung constant, M the number of the nearest neighbours, and R now the shortest interionic distance.

Put (5) and (6) into (4), we have

$$U = N \left[-\frac{2\alpha_m Z_+ Z_-}{R} + M \cdot V_{ol}^{+-}(R) + (\Delta E_+ + \Delta E_-)/2 \right]. \quad (7)$$

Therefore, the cohesive energy per pair of positive and negative ions of the crystal by ionic overlap-compression model is

$$\begin{aligned} E_{ioc} &= \frac{U}{N} \\ &= -\frac{2\alpha_m Z_+ Z_-}{R} + M \cdot V_{ol}^{+-}(R) + (\Delta E_+ + \Delta E_-)/2. \end{aligned} \quad (8)$$