徐祖耀文选

（续）

上海交通大学
材料科学与工程学院 编

The Selected Works *of* T.Y.Hsu (Continued)

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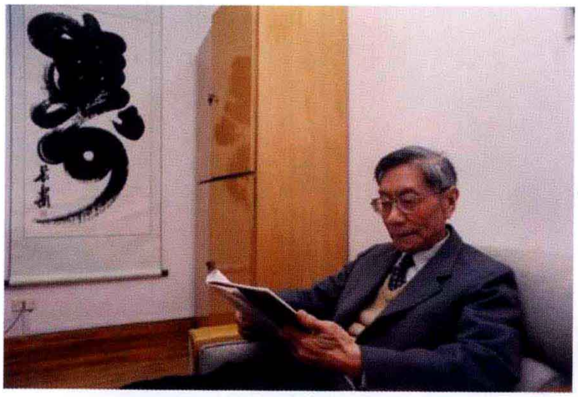
MARCH 2002, IN HIS OFFICE



Working in office

Working in office

2001-Discussion with his group members (From left to right: Prof. Jihua Zhang, Prof. Shipu Chen, Prof. T. Y. Hsu, Dr. Hongtao Zhu, Prof. Yonghua Rong and Dr. Zhenghong Guo)

2001-With colleagues in Haiyan, Zhejiang province (From left to right: Prof. Mingjuan Hu, Prof. T. Y. Hsu, Prof. Pinnan Zhou, Prof. Shipu Chen and Prof. Yonghua Rong)

2001-Resignment speech at conference of Shanghai Society for Heat Treatment after acting as the chairman since the birth of the Society in 1981. Left: Prof. Luopin Xu; Right: Academician Jiansheng Pan

2001-Accepted the celebration card for his 80th birthday from Prof. Luopin Xu(left), Lin Li(middle) and Xiaochun Wu(right) at the banquet in Shanghai

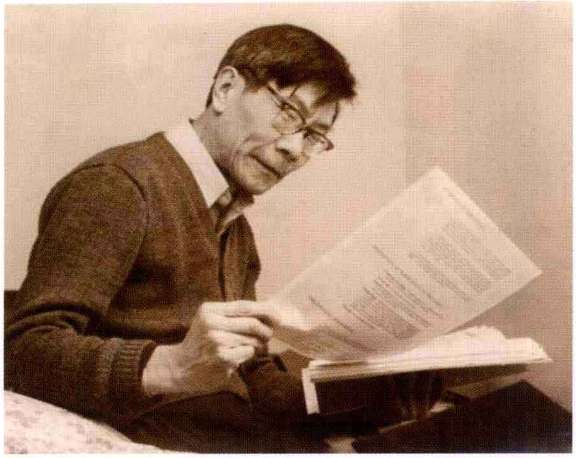
2000-Visited Taiwan and delivered four lectures in different universities

2000-Lecture on the Material for Engineering Applications, The 1st International Conference on Mechanical Engineering, Shanghai

2004-As the Congress Chairman of International Federation for Heat Treatment and Surface Engineering

2005-As the Co-Chairman of ICOMAT-05 and delivered plenary lecture in Shanghai

2005-Discussion with Prof. K. Shimizu (清水谦一) at the ICOMAT-05 in Shanghai



2005-Interviewed with a reporter about himself in newspaper Wenweipo published in Hong Kong.

2005-With his partial students and group members at the ICOMAT-05 in Shanghai

After obtaining the *Progress in Science and Technology Prize* by the Ho Leung Ho Lee Foundation in 2000

Statue of Prof. Hsu(left) in Statue Park of academician, his native Ningbo, Zhejiang province

Foreword

Professor T. Y. Hsu (Xu Zuyao) is a professor of School of Materials Science and Engineering (SMSE), Shanghai Jiao Tong University (SJTU). As a senior member of the Chinese Academy of Sciences (CAS), Prof. Hsu is a world—wide known materials scientist. Ten years ago, The Selected Works of T. Y. Hsu (Xu Zuyao), a collection of scientific publications of Prof. Hsu, was published by SMSE on occasion of his 80th birthday ceremony. It was my great honor to get a copy of the book later from him. After reading the book, I was very much encouraged by his spirit of devoting himself entirely into materials research and his significant achievements over the past decades.

With Prof. Hsu's kind recommendation, I was fortunately appointed as the dean of SMSE of SJTU during 2004—2007. With this post, I had plenty of opportunities to meet Prof. Hsu for academic discussions and for exchanging opinions on various aspects intensively. I was keenly aware of his rigorous scholarship and respectful virtue. On the occasion of his coming 90th birthday, SMSE of SJTU decided to publish a continuation of the collection reflecting his recent progress in materials research. As the head of Academic Committee of SMSE, I am greatly honored to write this Foreword in honor of Prof. Hsu's tremendous achievements in materials science and his great personality.

To honor 68 years of his professional career in research and teaching, the content of this continuation is composed of 68 English essays selected from his recent publications. These essays, combining with other essays and books as listed in appendix, cover a broad array of activities centering on the subject of phase transformation and its applications. Recognizing the excellent research works on shape memory materials, his group was awarded the Natural Science Prize of The Ministry of Education in 2001 (second class) and Progress Prize in Science and Technology of Shanghai Municipal Government in 2004 (second class). He and his group recently investigated structural stability of nanostructured materials by developing the thermodynamical criterion and physical model of martensitic/diffusional transformation. He investigated phase transformation under external stress, integration of plasticity forming and heat treatment processes, for developing advanced processes for energy—saving. His insight into the ultrahigh strength steel resulted in the launch of novel heat treatment manner of carbon steel, quenching—partitioning—tempering, based on original quenching & partitioning one. He proposed and refined potential research directions by writing review articles, communicated with scholars and engineers by delivering lectures in factories and other research institutes; He was invited to present lectures at Baosteel, Taiyuan Steel, Laiwu Steel, Central Iron and Steel Research Institute of China, Taiyuan University of Technology, China Distinguished Materials Scientist Forum at University of Science and Technology of Beijing and Institute of Metals Research of CAS, actively advocated to the service philosophy of science to society and the collaboration among industry, university and research unit. An important example was that he led SMSE of SJTU to visit Laiwu Steel and to establish the unified R&D center for high strength steel, of which he serves as the general director.

Professor Hsu has been throwing himself into the education reform. He has put the university and school forward of many valuable advices on curriculum and discipline planning and construction, considered the orientation of advanced educational policy. He not only supported other faculty members to write academic works, but also organized staffs to edit textbook for graduate students (including *Thermodynamics of Materials* which has been published and *Phase Transformation in Materials* which is in press) and handbook (including *Materials Characterization and Measurement Technology*, Vol. 26 of *Encyclopedia of China Materials Engineering*). He was awarded by the National Teaching Achievements (second class) and Teaching Achievements (first class) from Shanghai municipal government respectively in 2001.

Professor Hsu frequently attended (more than 10) domestic and international conferences as an invited or keynote speaker in the past 10 years. I should specially point out here that Shanghai won the bid of hosting the ICOMAT—2005 and the conference was held on schedule. Professor Hsu and Professor Liancheng Zhao have played key role for this success. Professor Peitikainen, who was the ex—chairman of ICOMAT—2002 in Helsinki, commented Shanghai conference was the most successful one in history. In 2005, as the only scholar from mainland China, he was invited as the member of the International Advisory Board of Solid—Solid Phase Transformation, and gave keynote address on the topic of bainitic transformation.

Being a younger generation and ex—colleague, I would like to take this opportunity to wish Professor Hsu a good health and longevity at the pressing of this continuation. Besides, I also would like to express sincere appreciation to the institutions and individuals who contributed to this collection.

(K. Lu)

Director of Institute of Metals Research

April 20, 2010

序

中国科学院院士徐祖耀教授是国际著名的材料科学家。10年前，值徐祖耀先生八十华诞之际，上海交通大学材料科学与工程学院举行了隆重的纪念活动，并出版《徐祖耀文选》以誌祝贺。承徐先生惠赠一本，得以窥见先生数十年潜心于材料科学事业之精神，并为其所取得的巨大成就所鼓舞。

近10年来，徐先生作为资深院士，强国之愿不减，依旧奋战在材料科学领域的前沿。在徐先生的推荐下，我有幸于2004～2007年间出任上海交通大学材料科学与工程学院院长一职，使我近年来有机会与徐先生进行更多深入的学术交流，进而能更真切地体认先生一生的学术思想与道德操守，并为之感佩与尊崇。今逢先生九十华诞，学院决定新撰《徐祖耀文选(续)》(以下简称《文选(续)》)，精选过去10年徐先生所发表的学术论文，编集成册交由科学出版社出版。作为上海交通大学材料科学与工程学院学术委员会主任，我十分荣幸受学院之邀为之作序，以表达我对先生数十年耕耘于材料科学领域的敬意。

《文选(续)》共载68篇英文学术论文，以表先生从教68年之意。这些论文，总合本书后所附近十年发表论文及出版书籍目录，完整涵盖了先生近期以相变原理及应用为中心，在多个研究方向上的辛勤探索与创造成果。例如，他领导的课题组因在形状记忆合金方面多年的研究积累，“铜基与铁基合金的马氏体相变及形状记忆合金效应”项目荣获2001年中国高等院校自然科学二等奖，“fcc－hcp的半热弹性马氏体相变及其诱导的形状记忆效应”项目荣获2004年上海市科学技术进步奖二等奖；他首先提出要关注纳米材料的结构稳定性问题，进而领导课题组发展了纳米材料结构稳定的热力学判据，以及发生马氏体相变和扩散相变的物理模型；他积极倡导先进高强钢的研究，关注应力作用下的相变，基于节能考虑提倡钢的塑形成型与热处理一体化，并指出其理论基础是多场(温度场、应力场或磁场)下的相变。在此基础上首倡Q-P-T工艺，以克服Q&P工艺的缺陷，领导课题组开发出新一类的超高强度结构钢。除此之外，他还撰写了大量综述性论文，阐明未来的研究方向，并到宝山钢铁厂、太原钢铁厂、莱芜钢铁厂、北京钢铁研究总院、太原理工大学、北京科技大学“中国材料名师讲坛”和中国科学院金属研究所等作学术交流，以倡导科学服务社会及产学研结合的理念。牵头建立校企合作项目以及成立联合实验室，亲任上海交通大学-莱芜钢铁厂高强度钢联合研发中心理事长。

除此以外，先生过去10年来仍旧关注教育改革的进展，多次对学校与学院学科建设与课程设置提出意见，思考材料科学与工程专业未来的发展方向。他不仅鼓励其他教师著书立说，而且积极组织编写研究生教材(包括由他主编并已出版的《材料热力学》和正付梓印刷的《材料中的相变》)，以及手册类图书[在已出版的《中国材料工程大典》(26卷)和《材料表征与测试技术》任主编之一]，并于2001年获国家级教学成果奖二等奖和2001年上海市教学成果一等奖。

多年来，先生积极活跃于国内与国际学术舞台，他曾在国际学术会议上做特邀报告或主题报告十余次。他与赵连城院士争取并成功在上海举办了2005年国际马氏体相变会议，得到国际同行的高度评价，上届会议主席彼蒂凯依(J. Peitikainen)教授认为该次会议是迄今为止办得最成功的一次会议。2005年应邀出任国际固态相变会议顾问委员会委员(大陆仅此一名)和做关于贝氏体相变的特邀报告。

值此《文选(续)》即将出版之际，作为曾经的同事及晚辈，谨愿先生健康长寿。此外，我也还以个人名义对本文选出版做出贡献的个人与团体表示真诚的谢意。

是为序。

中国科学院金属研究所所长

中国科学院院士

2010年4月20日

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Ⅰ. Martensitic and Bainitic Transformations

Materials science communication

Group theory analyses of transition structures related to the $\gamma \rightarrow \varepsilon$ transformation in Fe–Mn–Si based alloys

J.F. Wan*, S.P. Chen, T.Y. Hsu (Xu Zuyao)

School of Materials Science and Engineering, Shanghai Jiao Tong University, Shanghai 200030, PR China

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Abstract

The fcc(γ) $\rightarrow$ hcp(ε) martensitic transformation in Fe–Mn–Si based shape memory alloys proceeds through a stacking fault mechanism. In the present paper, the symmetry characteristics of stacking faults are described by using the layer group theory, indicating that the intrinsic SF belongs to $P_{\bar{6}2m}$ and the extrinsic fault to P_{321}. The fault tetrahedron exhibits some sort of symmetry too. According to various repeating structures of the close-packed planes, transition states of the formed martensite are listed and exemplified. A thermodynamic method is proposed to calculate their chemical free energies and evaluate their stabilities which are in the order of 2H > 4H > 5H > 6H > 8H.

Keywords: Group theory analysis; Transition structures; Stacking fault mechanism

1. Introduction

It is well known that the $\gamma \rightarrow \varepsilon$ transformation in Fe–Mn–Si based shape memory alloys is associated with stacking faults (SF), while the stacking fault tetrahedron (SFT) plays an important role in the SF initiation [1,2]. The stacking faults have been extensively investigated on various aspects, such as the thermodynamic calculation of SF energy [3,4], the XRD measurement of SF probability (P_{sf}) [5] and the CTEM and HRTEM observations of SF and SFT [6,7]. However, only little work was done on their symmetry characteristics till now. On the other hand, thermomechanical training as an effective method to improve the shape memory effect (SME) may lead to formation of transition phases of which some have been examined by internal friction experiment in Fe–26.4Mn–6.0Si–5.2Cr alloy [8] and characterized by TEM in Fe–30Mn–6Si alloy [9], but the others are still not identified. The group theory will be used to describe the symmetry characteristics of the SF and SFT, to predict the possible transition phases in Fe–Mn–Si based alloys and to evaluate their stabilities based on thermodynamic consideration.

* Corresponding author.

2. Symmetry of planar stacking faults

Stacking fault as a kind of planar defects is not a simple plane, but actually is a three-dimensional-structured plane with two-dimensional period. Because of its very low SFE (several mJ/m^2) and, thus, its rather wide extension in Fe–Mn–Si based alloys, the stacking fault belongs to this kind of specific plane. Therefore, the layer group in symmetry groups can be suitably used for studying the symmetry characteristics of such stacking faults.

2.1. Layer group

Crystal symmetry group includes point group, plane group, layer group and space group besides staff group, color group and so on. Among them, layer group describes the symmetry group of two-plane objects with double-layer structure which is different from two-dimensional plane group. For the two-dimension situation, 17 kinds of plane groups can be deduced by means of operations including rotation transformation (one- to six-fold axes except the five-fold one), reflected plane (m) and translation. When a single plane changes into double, an inversion center (i) and a rotating inversion as new operations lead to 80 kinds of layer groups with the definition of space group on the basis of plane group. All these layer groups attributing to four crystal systems (rectangle, rhemble, tetragonal and hexagonal)

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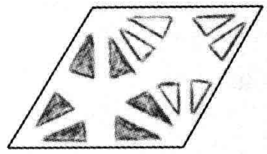

Fig. 1. Layer group $P_{\bar{3}ml}$ of AB.

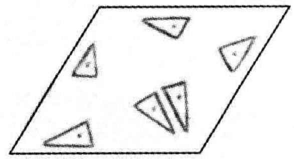

Fig. 3. Layer group of the intrinsic SF.

can characterize a series of crystals with layer-like structure, such as graphite, pyrophylite, honeycomb and biomembrane.

A {1 1 1} plane in fcc structure has the point group 6 mm and the space group P_{6mm}. The space group of a double {1 1 1} plane in AB stacking sequence with an inversion center (*i*) is of the structure being a special layer group $P_{\bar{3}ml}$ (Fig. 1), while the layer group of two AA-stacking planes constructing reversal domain and introducing a reflected plane (*m*) is $P_{\bar{6}m2}$ as shown in Fig. 2. The symmetry of $P_{\bar{6}m2}$ is obviously prior to that of $P_{\bar{3}ml}$ and, therefore, AA and AB can be distinguished by layer group.

2.2. Symmetry of stacking faults

Face-centered cubic crystal as a close-packed structure can be constructed by stacking the {1 1 1} planes in the order of ABCABC.... The stacking fault in this structure is always lying in the {1 1 1} plane. There exist two classical types of SF as follows: (1) intrinsic SF, being equal to draw out a close-packed plane from the planes in normal order; and (2) extrinsic SF, seeming to insert a lose-packed plane or to cascade two intrinsic SFs. SF in fcc could also be considered as a thin piece of close-packed hexagonal structure. Therefore, it is reasonable to associate the symmetry of intrinsic (or extrinsic) SF with that of a single piece of hcp structure-ABA (or a double hcp structure-ABACA). In order to apply the layer group to the SFs with three- or five-layer structure, they can be dealt with equivalently.

Intrinsic SF-ABA is piled up by AB and BA under the condition of same symmetry,

ABA = AB + BA

Then, AB or BA is able to be considered as a special single layer with the point group 3*m* and the plane group P_{31m}, which is different from those of a single layer A or B. A new symmetry operation, reflected plane (*m*)-B atomic plane, will be introduced after AB and BA being connected. Therefore, the layer group of ABA becomes $P_{\bar{6}2m}$ (Fig. 3). The similar operations are used to deal with the extrinsic SF (ABACA) and their relationship is shown as

ABACA = (ABA) + (ACA) = (AB + BA) + (AC + CA).

The plane group of ABA and ACA, both as one layer, is P_{31m}. For the ABC layer in extrinsic SF, B is inversely symmetrical to C about A plane which is also the inversion center for ABA and ACA and, hence, the symmetry characteristics of extrinsic SF should be of layer group P_{321}, as shown in Fig. 4. Referring to the extrinsic SF, the symmetry of a twin structure ABCBA can be deduced by considering ABC and CBA as one layer with plane group of P_3 and they are symmetrical to each other about *C* plane. Based on these features, the layer group of a twin should be $P_{\bar{6}2m}$, same as that of ABA.

3. Symmetry of stacking fault tetrahedron

Stacking fault tetrahedron was observed in the alloys such as Au based and Co–Ni with low SFE about 32 and 16 mJ/m^2, respectively [10,11]. When a specimen of Fe–Mn–Si alloy with the SFE less than 10 mJ/m^2 was quenched to room temperature, the supersaturated vacancies collapsed to form tetrahedrons. Existing the same angles among four {1 1 1} planes, the tetrahedron is an orthotetrahedron with a bottom of vacancy plate and three identical sides of extended SF plane. If the bottom is also considered as an SF plane, the tetrahedron consists of four sides.

The tetrahedron with three SF sides has symmetry elements of a third axis (C_3) perpendicular to the bottom plane

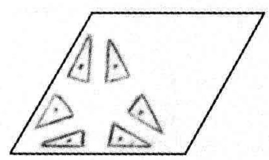

Fig. 2. Layer group $P_{\bar{6}m2}$ of AA.

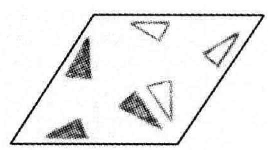

Fig. 4. Layer group of the extrinsic SF.