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目 录

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论文证明



A cluster-plus-glue-atom composition design approach designated for multi-principal element alloys

Xuan Liu, Hui-Bin Ke*[✉], Liang Wang, Yao-Jian Liang, Lin-Jing Wang, Ben-Peng Wang, Lu Wang, Qun-Bo Fan, Yun-Fei Xue

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Abstract Multi-principal element alloys (MPEAs) have shown extraordinary properties in different fields. However, the composition design of MPEAs is still challenging due to the complicated interactions among principal elements (PEs), and even more challenging with precipitates formation. Precipitation can be either beneficial or detrimental in alloys, thus it is important to control precipitates formation on purpose during alloy design. In this work, cluster-plus-glue-atom model (CGM) composition design method which is usually used to describe short-range order in traditional alloys has been successfully extended to MPEAs for precipitation design. The key challenge of extending CGM to MPEAs is the determination of center atom since there are no solvent or solute in MPEAs. Research has found that the element type of center atom was related not only with chemical affinity, but also with atomic volume difference in MPEAs, which has inevitable effect on atomic arrangement. Based on experimental data of MPEAs with precipitates, it was found that elements with either stronger chemical affinity or larger volume difference with other PEs would occupy the center site of clusters. Therefore, a cluster index (P_C), which considers both chemical affinity and atomic volume factors, was proposed to assist the determination of center atom in MPEAs. Based on the approach, a solid-solution Zr-Ti-V-Nb-Al BCC alloy was obtained by inhibiting the

precipitation, while precipitation-strengthened Al-Cr-Fe-Ni-V FCC alloy and Al-Co-Cr-Fe-Ni BCC alloy were designed by promoting the precipitation. Corresponding experimental results demonstrated that the approach could provide a relatively simple and accurate prediction of precipitation and the compositions of precipitations were in line with PEs in cluster in MPEAs. The research may open an effective way for composition design of MPEAs with desired phase structure.

Keywords Multi-principal element alloy (MPEA); Composition design; Phase structure; Cluster-plus-glue-atom model (CGM)

1 Introduction

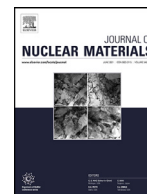
In recent years, multi-principal element alloys (MPEAs) have attracted much interest [1–5] due to their excellent performance [6–13]. Performance of alloys are closely related to their phase structures and vast efforts have been devoted to phase prediction in MPEAs [14–22].

At present, the most frequently used phase prediction methods for MPEAs are empirical criteria and CALPHAD (CALculation of PHase Diagram). Empirical criteria such as atomic size differences (δ) [14, 15], electronegativity difference ($\Delta\chi$) [16], valance electron concentration (VEC) [17] and thermodynamic parameters (Ω) [18] are usually obtained by summarizing reported data, resulting in the limitation on alloy system. Similarly, CALPHAD relies on existing database, which mostly contain binary and limited ternary alloy systems, since the database for higher-order alloy systems is grossly imperfect yet [19–22]. Furthermore, empirical criteria and CALPHAD are useful in

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Helium interaction with solutes and impurities in neutron-irradiated nanostructured ferritic alloys: A first principles study

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ABSTRACT

Density functional theory (DFT) calculations are performed to explore the binding between He and alloying solutes, impurities, and transmutation products expected in neutron irradiated nanostructured ferritic alloys (NFAs), here 14YWT is taken as an example. Elements that exhibit significant binding (attraction) with an interstitial He are: Y (binding energy = 0.46 eV), Mg (0.32), O (0.33), Ti (0.16), and C (0.15). Those that provide significant binding to a substitutional He are: O (1.44), Y (1.24), N (0.73), H (0.56), Mg (0.52), Ti (0.34), Si (0.34), C (0.33), Al (0.32), Ni (0.26), Ta (0.23), and Mn (0.16). The presence of these elements in Fe matrix could reduce the transport of He towards oxide particles, dislocations, and internal boundaries, and could promote He bubble nucleation in the matrix. For convenience, we compile existing binding energy data of He with He_n and He_nV (He-vacancy) clusters. Dissociation pathway analysis reveals that, in general, the most likely dissociation of a He_nV cluster is by a sequential emission of individual He atoms. Furthermore, larger bubbles are more prone to dissociation than smaller ones. In addition, we estimate the binding energy (segregation energy) of He in bulk $\text{Y}_2\text{Ti}_2\text{O}_7$ (YTO) single crystal, YTO/Fe interface, and YTO particle embedded in Fe, with respect to interstitial He in Fe, from existing formation energies of He in these structures. We also compile available data of He binding with Fe self-interstitial atom (SIA), SIA clusters, and edge and screw dislocations. Note that given the absence of DFT data, the binding with SIA clusters and dislocations are gathered from simulations with empirical potentials. The data presented in this paper is important to inform multiscale simulations of He bubble accumulation.

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1. Introduction

Deuterium-tritium fusion reaction produces high energy ~ 14 MeV neutrons that create significant atomic displacements (vacancies and interstitials) through elastic collisions, and He and H gases through inelastic collisions with the atoms in first wall and blanket structures. The standardized metric for quantifying the displacement damage is displacements per atom (dpa) [1]. In a fusion reactor, e.g. based on ARIES-ACT2 design concept with F82H alloy as the structural material, the peak damage at the first wall is expected to be ~ 21 dpa/FPY while the peak He gas production from transmutation is ~ 225 appm/FPY (FPY stands for full peak year) [2]. The ~ 14 MeV neutron radiation generates approximately 50 to 100 times higher He/dpa in materials such as martensitic/ferritic steels compared to neutron radiation of fission reactors [3]. Hence the ferritic/martensitic steels, that are being used in nuclear fission power plants, are incapable of withstanding the large dpa and He production expected in fusion reactors.

Reduced activation ferritic/martensitic (RAFM) steels were developed in early 1980s by replacing Mo with W and Nb with Ta [4]. Currently, RAFM steels such as F82H, EUROFER97, INRAFM and CLAM, are the most technologically matured options for fusion blanket structural materials with excellent properties, such as, high thermal conductivity, low thermal expansion coefficient, and relatively low void swelling during neutron irradiation compared to alternative structural materials [5]. However, the operating temperatures of the RAFM steels are $< 500 - 600^\circ\text{C}$. This temperature limit was improved without degrading the advantages inherent of RAFM steels by strengthening the Fe matrix with dispersion of fine oxide particles [3]. These steels are called oxide dispersion strengthened (ODS) steels. Nanostructured ferritic alloys (NFAs) are a subset of ODS steels that contain a high number density ($> 10^{23}$ particles/ m^3) of ultrafine (< 3 nm diameter) particles. Dislocation pinning by these nanoparticles improves the high-temperature thermal creep strength of NFAs. In addition, NFAs exhibit much improved void swelling than RAFM steels due to efficient trapping of He atoms by the nanoparticles. The science, development, and applications of these NFAs are reviewed in several articles [3,6–8].

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Review

Christopher D. Taylor* and Huibin Ke

Investigations of the intrinsic corrosion and hydrogen susceptibility of metals and alloys using density functional theory

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Abstract: Mechanisms for materials degradation are usually inferred from electrochemical measurements and characterization performed before, during, and after exposure testing and/or failure analysis of service materials. Predicting corrosion and other materials degradation modes, such as hydrogen-assisted cracking, from first-principles has generally been limited to thermodynamic predictions from Pourbaix or Ellingham diagrams and the Galvanic series. Using electronic structure calculations, modern first-principles methods can predict *ab initio* the key rate-controlling processes for corrosion and hydrogen susceptibility as a function of pH, potential, and solution chemistry, and materials composition and microstructure. Herein we review density functional theory (DFT) approaches for studying the electrochemical reactions occurring on fresh metal and alloy surfaces related to environmentally assisted cracking and localized corrosion/pitting. Predicted changes in surface chemistry as a function of the environment were correlated against experimental crack growth rate data obtained for alloys 718, 725, and pipeline steel under electrochemical control. We also review the application of the method to study the effects of alloying on the chloride susceptibility of stainless steels and Ni–Cr-based corrosion-resistant alloys. Perspectives for improving the model are given, and extending it to future fields of application in corrosion science and engineering.

Keywords: density functional theory; electrochemistry; hydrogen adsorption; localized corrosion; surface adsorption.

1 Introduction

Physics-based simulation of materials aging and degradation through the mechanisms of corrosion and hydrogen embrittlement remains a challenging field of research (Barrera et al. 2018; Taylor 2015). Such research is motivated by the necessity for decision-makers in materials engineering and design to develop new materials that are more robust under a variety of environments, to establish fitness for service criteria, and to extend the lifetime of aging structures (Cordeiro et al. 2020; Taylor et al. 2018c). Credible models can help augment and interpret the often-limited set of relevant historical and experimental databases that typically inform such decision-making processes (Melchers 2019). Such models can fall into two generic categories: empirical models, with sometimes (but not always) physically motivated functional forms that are parameterized to laboratory and/or field data (Feliu et al. 1993a, 1993b; Melchers 2019; Mendoza and Corvo 2000; Oesch and Faller 1997); and first-principles models that are physically motivated and parameterized only by fundamental physical constants (Huang et al. 2019; Lin et al. 1981; Sharland 1987; Taylor 2015; Taylor et al. 2018c).

The development of first-principles models for corrosion and hydrogen embrittlement will require a careful reconstruction of the key physicochemical processes that contribute to those phenomena (Gunasegaram et al. 2014). These processes include mass-transport from the environment to the near-surface region; chemical and electrochemical reactions at the electrified interface between the material and solution; compositional and microstructural changes in the material itself; interactions of solutes and surfaces with static and dynamic strain fields in the material; and formation and evolution of surface films and scales (Anderko et al. 2008, 2014, 2015; Barrera et al. 2018; Rice and Wang 1989; Shibata 2007; Tehranchi et al. 2020).

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Method to identify the phase structures of high entropy alloys with modified lattice distortion enthalpy

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Material calculation

ABSTRACT

Severe lattice distortion is one of important characteristics of high entropy alloys (HEAs) and exercises considerable influence over phase structures, and atomic volume V is thought to be the key factor for lattice distortion. In the present work, the calculation of V was modified by taking the stacking density effects into consideration, and the calculation of lattice distortion enthalpy (ΔH_{LD}) caused by elastic lattice distortion for HEAs was optimized accordingly. With this method, two phase structure formation rules were proposed: valence electron concentration (VEC) $-\Delta H_{LD}$ rule for crystal structure of solid solution and chemical enthalpy (ΔH_{chem}) $-\Delta H_{LD}$ rule for phase composition. The prediction effect of these two rules were verified by analyzing 100 existing HEAs, and the intrinsic effect of lattice elastic distortion on the phase formation of HEAs were discussed. The results of the research would be helpful in the composition design of HEAs.

1. Introduction

The proposing of high entropy alloys (HEAs) has broken the traditional alloy design concept and attracted considerable attention [1–13]. As the element interaction in HEAs is more complex than traditional alloys, it became harder for researchers to make quantitative and well-targeted design. Therefore, prediction of phase structures is a key research for HEAs composition design, which could not only improve quality, but also reduce cycle time and lower costs.

Two aspects are mainly included in the phase prediction research: phase composition prediction and crystal structure prediction of single-phase solid-solution (SS). The former means to predict what phases would be included in the alloy, such as SS, intermetallic compounds (IM) and amorphous phase. During the early stage of HEAs, the configurational entropy ΔS_{con} was regarded as the dominating parameter responsible for the stability of SS structure in HEAs [14,15], but deeper research indicated that ΔS_{con} is not enough [16]. Two factors were later proposed to predict the phase composition: enthalpy of mixing (ΔH_{mix}) [17] and the electronegativity mismatch ($\Delta\chi$) [18]. The crystal structure prediction study aims to make a prediction about which lattice structure will be formed in SS, such as body-centered cubic (BCC), face-centered

cubic (FCC) and hexagonal close-packed (HCP). the most commonly used parameter is valence electron concentration (VEC): FCC crystalline structures will be formed when $VEC \geq 8$, and BCC structures for $VEC < 6.7$ [19]. These parameters, ΔH_{mix} , $\Delta\chi$ and VEC were derived from traditional alloys and seem the precision is not sufficient for HEAs due to its severe lattice distortion [21–23]. There can be no doubt that the lattice distortion enthalpy resulting from lattice distortion plays a crucial role in phase formation of HEAs. At the beginning of the study, the size mismatch δ was used to characterize the size difference between principal elements, Researchers found that when alloys having similar ΔH_{mix} or $\Delta\chi$, the combination with δ will be helpful to identify complex phase structures [17]. After that, elastic distortion energy was proposed, as the atomic volume can better reflect the distortion degree of crystal structure [2,24–27].

The method proposed by Melnick [16] provided concise approach to calculate lattice elastic-strain energy. One of the crucial parameters in Melnick's approach is local atomic volumes V and it was calculated by divide the molar volume by Avogadro constant. However, it is noteworthy that there is slight difference between atomic volumes of different crystal structures: the bulk volume is the same across the various crystal structures, but the packing efficiency (coordination

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委托检索信息

委托人: 柯慧彬

委托人单位: 北京理工大学

委托查询时间范围: 2021~2024 年

检索数据库

1. 美国《科学引文索引》(SCI-EXPANDED, 网络版)
2. 美国《期刊引用报告》(JCR, 网络版)
3. 中科院 SCI 分区表(网络版)

检索结果

本次检索根据委托人 柯慧彬 所提供的论文目录及其检索要求, 通过对上面的数据库进行检索, 检索结果如下:

1. 在美国《科学引文索引》(SCI-EXPANDED, 网络版)中收录 4 篇。
2. 美国《期刊引用报告》(JCR, 网络版)收录 4 种期刊。
3. 中科院 SCI 分区表(网络版)收录 4 种期刊。

(注: 关于他引和自引的区分, 本证明所采用的方法是: 文献被除第一作者及合作者以外其他人的引用为他引)

(检索结果详见附件)

特此证明!

检索人: 韩萌萌
查证单位: 教育部科技查新工作站(L27)
北京理工大学查新检索咨询中心
2024年03月12日

作者论文情况概览

序号	标题/作者/来源	收录情况	贡献情况
1	<p>A cluster-plus-glue-atom composition design approach designated for multi-principal element alloys</p> <p>作者:Liu, X (Liu, Xuan);Ke, HB (Ke, Hui-Bin);Wang, L (Wang, Liang);Liang, YJ (Liang, Yao-Jian);Wang, LJ (Wang, Lin-Jing);Wang, BP (Wang, Ben-Peng);Wang, L (Wang, Lu);Fan, QB (Fan, Qun-Bo);Xue, YF (Xue, Yun-Fei)</p> <p>来源: RARE METALS 卷: 41 期: 11 页: 3839-3849 出版年: 2022 文献类型: Article; Early Access</p> <p>Accession Number:SCIE: WOS:000852333300001</p>	SCIE	通讯作者
2	<p>Helium interaction with solutes and impurities in neutron-irradiated nanostructured ferritic alloys: A first principles study</p> <p>作者:Pitike, KC (Pitike, Krishna Chaitanya);Ke, HB (Ke, Huibin);Edwards, DJ (Edwards, Danny J.);Setyawan, W (Setyawan, Wahyu)</p> <p>来源: JOURNAL OF NUCLEAR MATERIALS 卷: 566 出版年: 2022 文献类型: Article; Early Access</p> <p>Accession Number:SCIE: WOS:000805635200006</p>	SCIE	
3	<p>Investigations of the intrinsic corrosion and hydrogen susceptibility of metals and alloys using density functional theory</p> <p>作者:Taylor, CD (Taylor, Christopher D.);Ke, HB (Ke, Huibin)</p> <p>来源: CORROSION REVIEWS 卷: 39 期: 3 页: 177-209 出版年: 2021 文献类型: Review</p> <p>Accession Number:SCIE: WOS:000656866600001</p>	SCIE	
4	<p>Method to identify the phase structures of high entropy alloys with modified lattice distortion enthalpy</p> <p>作者:Liu, X (Liu, Xuan);Jia, NN (Jia, Nannan);Chen, SS (Chen, Songshen);Wang, L (Wang, Liang);Ke, HB (Ke, Huibin);Jin, K (Jin, Ke);Wang, BP (Wang, Benpeng);Wang, L (Wang, Lu);Fan, QB (Fan, Qunbo);Xue, YF (Xue, Yunfei)</p> <p>来源: MATERIALS TODAY COMMUNICATIONS 卷: 29 出版年: 2021 文献类型: Article; Early Access</p> <p>Accession Number:SCIE: WOS:000702718300005</p>	SCIE	

附件一:

收录详细情况

1. Title: A cluster-plus-glue-atom composition design approach designated for multi-principal element alloys

Author(s): Liu, X (Liu, Xuan);Ke, HB (Ke, Hui-Bin);Wang, L (Wang, Liang);Liang, YJ (Liang, Yao-Jian);Wang, LJ (Wang, Lin-Jing);Wang, BP (Wang, Ben-Peng);Wang, L (Wang, Lu);Fan, QB (Fan, Qun-Bo);Xue, YF (Xue, Yun-Fei)

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作者地址: ["[Liu, Xuan; Ke, Hui-Bin; Liang, Yao-Jian; Wang, Lin-Jing; Wang, Ben-Peng; Wang, Lu; Fan, Qun-Bo; Xue, Yun-Fei] Beijing Inst Technol, Sch Mat Sci & Engn, Beijing 100081, Peoples R China", "[Wang, Liang] Beijing Inst Technol, Inst Adv Struct Technol, Beijing 100081, Peoples R China"]

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2. Title: Helium interaction with solutes and impurities in neutron-irradiated nanostructured ferritic alloys: A first principles study

Author(s): Pitike, KC (Pitike, Krishna Chaitanya);Ke, HB (Ke, Huibin);Edwards, DJ (Edwards, Danny J.);Setyawan, W (Setyawan, Wahyu)

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ISSN: 0022-3115

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3. Title: Investigations of the intrinsic corrosion and hydrogen susceptibility of metals and alloys using density functional theory

Author(s): Taylor, CD (Taylor, Christopher D.);Ke, HB (Ke, Huibin)

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通讯作者: ["[Taylor, Christopher D.] (corresponding author), DNV GL USA, Mat Technol & Dev Sect, Pipeline Serv, Dublin, OH 43017 USA", "[Taylor, Christopher D.] (corresponding author), Ohio State Univ, Fontana Corros Ctr, Dept Mat Sci & Engr, Columbus, OH 43210 USA"]

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4. Title: Method to identify the phase structures of high entropy alloys with modified lattice distortion enthalpy

Author(s): Liu, X (Liu, Xuan); Jia, NN (Jia, Nannan); Chen, SS (Chen, Songshen); Wang, L (Wang, Liang); Ke, HB (Ke, Huibin); Jin, K (Jin, Ke); Wang, BP (Wang, Benpeng); Wang, L (Wang, Lu); Fan, QB (Fan, Qunbo); Xue, YF (Xue, Yunfei)

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通讯作者: ["[Xue, Yunfei] (corresponding author), Beijing Inst Technol, Sch Mat Sci & Engr, Beijing 100081, Peoples R China"]

作者地址: ["[Liu, Xuan; Jia, Nannan; Chen, Songshen; Ke, Huibin; Wang, Benpeng; Wang, Lu; Fan, Qunbo; Xue, Yunfei] Beijing Inst Technol, Sch Mat Sci & Engr, Beijing 100081, Peoples R China", "[Wang, Liang] Beijing Inst Technol, Inst Adv Struct Technol, Beijing 100081, Peoples R China", "[Jin, Ke] Beijing Inst Technol, Adv Res Inst Multidisciplinary Sci, Beijing 100081, Peoples R China"]

eISSN: 2352-4928

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附件二:

美国《期刊引用报告》(JCR)收录情况

1. 刊名: RARE METALS

ISSN: 1001-0521

2022 年影响因子: 8.8

JCR® 类别	类别中的排序	JCR 分区
MATERIALS SCIENCE, MULTIDISCIPLINARY	62/344	Q1
METALLURGY & METALLURGICAL ENGINEERING	4/79	Q1

2. 刊名: Journal of Nuclear Materials

ISSN: 0022-3115

2022 年影响因子: 3.1

JCR® 类别	类别中的排序	JCR 分区
MATERIALS SCIENCE, MULTIDISCIPLINARY	188/344	Q3
NUCLEAR SCIENCE & TECHNOLOGY	2/34	Q1

3. 刊名: CORROSION REVIEWS

ISSN: 0334-6005

2022 年影响因子: 3.2

JCR® 类别	类别中的排序	JCR 分区
MATERIALS SCIENCE, COATINGS & FILMS	10/21	Q2
METALLURGY & METALLURGICAL ENGINEERING	22/79	Q2
ELECTROCHEMISTRY	18/30	Q3

4. 刊名: Materials Today Communications

ISSN: 2352-4928

2022 年影响因子: 3.8

JCR® 类别	类别中的排序	JCR 分区
MATERIALS SCIENCE, MULTIDISCIPLINARY	153/344	Q2

附件三:

中科院 SCI 分区表 (网络版) 收录情况

1. 大类情况

期刊全称	ISSN	所属大类	大类分区	Top 期刊
RARE METALS	1001-0521	工程技术	2	否

小类情况

期刊全称	ISSN	所属小类	小类分区
RARE METALS	1001-0521	MATERIALS SCIENCE, MULTIDISCIPLINARY 材料科学: 综合	2
RARE METALS	1001-0521	METALLURGY & METALLURGICAL ENGINEERING 冶金工程	2

2. 大类情况

期刊全称	ISSN	所属大类	大类分区	Top 期刊
JOURNAL OF NUCLEAR MATERIALS	0022-3115	工程技术	3	是

小类情况

期刊全称	ISSN	所属小类	小类分区
JOURNAL OF NUCLEAR MATERIALS	0022-3115	MATERIALS SCIENCE, MULTIDISCIPLINARY 材料科学: 综合	4
JOURNAL OF NUCLEAR MATERIALS	0022-3115	NUCLEAR SCIENCE & TECHNOLOGY 核科学技术	1

3. 大类情况

期刊全称	ISSN	所属大类	大类分区	Top 期刊
CORROSION REVIEWS	0334-6005	工程技术	4	否

小类情况

期刊全称	ISSN	所属小类	小类分区
CORROSION REVIEWS	0334-6005	ELECTROCHEMISTRY 电化学	4
CORROSION REVIEWS	0334-6005	MATERIALS SCIENCE, COATINGS & FILMS 材料科学: 膜	4
CORROSION REVIEWS	0334-6005	METALLURGY & METALLURGICAL ENGINEERING 冶金工	3

		程	
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4. 大类情况

期刊全称	ISSN	所属大类	大类分区	Top 期刊
Materials Today Communications	2352-4928	工程技术	3	否

小类情况

期刊全称	ISSN	所属小类	小类分区
Materials Today Communications	2352-4928	MATERIALS SCIENCE, MULTIDISCIPLINARY 材料科学: 综合	4



10.24

项目证明

北京理工大学人力资源部

证明

柯慧彬，女，汉族，1989年11月24日生，身份证号码：
2[REDACTED]1，2021年获批火炬计划攻关项目青年项目。

特此证明。

北京理工大学人力资源部

2024年3月13日



[REDACTED]

[REDACTED]

基础加强计划重点基础研究项目 合同书

项目名称: [REDACTED] 控焯合金设计及其制造技术

项目牵头单位: 北京理工大学

项目负责人: 薛云飞

合同起止时间: 2021年11月至2025年11月

中央军委科学技术委员会制

[REDACTED]

项目分解说明

一、项目总体情况表

项目编号	项目名称	负责单位	负责人	身份证号	职务	职称	手机	单位机关联系人	机关联系人联系电话
		北京理工大学	薛云飞		无	教授		黄凯旋	01068912325

二、项目分解表

课题编号	课题名称	负责单位	负责人	身份证号	职务	职称	手机	所有参研单位
课题 1		北京理工大学	柯慧彬					
课题 2								

1. 课题经费分配表

课题 \ 节点		金额单位：万元			
		合同签订	中期评估	合同验收	合计
课题 1		100	80	20	200

202120943215

密级：公开

国防基础科研计划
项目任务书

项目编号：WDZC2021-2

项目名称：含能高熵合金燃烧释能与材料基础本征参数相关性研究

项目类型：一般项目

所属专题：实验室稳定支持专题

起止时间：2021年—2023年

经费概算： 28 万元 （其中国拨：28 万元）

项目负责人：柯慧彬

联系电话：010-68912709, 17610268911

（主）承研单位：北京理工大学（冲击环境材料技术重点实验室）

通讯地址：北京市海淀区中关村南大街5号，100081

主管单位：工业和信息化部

填报日期：2021年06月25日

国家国防科技工业局制

国防基础科研项目
主承研单位诚信承诺书

我单位已仔细阅读国防基础科研计划相关的管理办法，理解其有关规定和要求，现郑重承诺：

项目材料真实、可靠，所申报的项目未列入国家或军队其他科研计划，申报渠道唯一。对因申报内容失实或违反有关规定所造成的后果，我单位愿承担相关责任。

项目负责人：（签字）柯慧彬

主承研单位：（盖章）

主管单位部门：（盖章）

2021年8月10日



密级：公开

北京理工大学科技创新计划

前沿交叉与学科创新专项计划

项目任务书

项目名称：含能高熵合金燃烧性能与可计算材料本征参数的关联机制研究

培育目标：国家自然科学基金优秀青年科学基金项目（海外）

国民行业代码：M7510

学科名称：材料科学-计算材料学

学科代码：4301035

负责人：柯慧彬 所在单位：材料学院

资助经费：30万 执行年限：2021年1月~2021年12月

填表日期： 年 月 日

北京理工大学

专利证明

证书号第6489635号



发明专利证书

发明名称：一种具有燃烧微爆特性的AlTiZr基多主元合金粉的制备方法

发明人：王本鹏;柯慧彬;薛云飞

专利号：ZL 2022 1 0682285.6

专利申请日：2022年06月15日

专利权人：北京理工大学

地址：100081 北京市海淀区中关村南大街5号

授权公告日：2023年11月17日

授权公告号：CN 115121800 B

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局长
申长雨

申长雨

2023年11月17日

特邀报告证明



中国腐蚀与防护学会
Chinese Society for Corrosion and Protection

Certificate of Appreciation

presented to



KE Huibin

In Recognition for the

Invited Lecture

19th Asian Pacific Corrosion Control Conference

16th-18th November 2023

Guangzhou, China

Prof. LI Xiaogang
Conference Chair



Chinese Society for
Corrosion and Protection

其他奖励



荣誉证书

柯慧彬同志：

获“师缘·北理”庆祝第38个
教师节暨教师表彰大会优秀人才类
表彰。

特颁此证，以为纪念。

书记：

校长：

2022年9月2日

