



太原科技大学

# 英语论文写作 学习心得体会

学 院\_\_\_\_\_材料科学与工程\_\_\_\_\_  
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# 《英文论文写作》学习心得体会

## 一、资料收集

1. 阅读大量相关博士论文、该研究方向的前沿期刊、学术会议文献集等，对该研究方向有一个宏观的整体认识了解。

2. 通过 CARS 校外访问知网、万方、爱思唯尔、Springer 等数据库资源。

## 二、论文题目

1. 不应过长或过短，一般为 8~15 个实词（介词和连词除外）。
2. 论文题目一般为名词，不能采用动宾短语或其他句型。
3. 概括要尽可能精准，尽量突出论文中的重要内容，避免题目空泛和语法错误。

举例如下：

(1) 论文题目 “An Interatomic Potential of Li-Mn-O System and Molecular Dynamics Simulations on Li Diffusion in Spinel  $\text{Li}_{1-x}\text{Mn}_2\text{O}_4$ ”（出自 Lee E, Lee K R, Lee B J. *An Interatomic Potential of Li-Mn-O System and Molecular Dynamics Simulations on Li Diffusion in Spinel  $\text{Li}_{1-x}\text{Mn}_2\text{O}_4$* [J]. *The Journal of Physical Chemistry C*, 2017, 121(24).）

(2) 论文题目 “Calculation of native defect energies in  $\alpha\text{-Al}_2\text{O}_3$  and  $\alpha\text{-Cr}_2\text{O}_3$  using a modified Matsui potential”（出自 Sun J, Stirner T, Matthews A. *Calculation of native defect energies in  $\alpha\text{-Al}_2\text{O}_3$  and  $\alpha\text{-Cr}_2\text{O}_3$  using a modified Matsui potential*[J]. *Surface and Coatings Technology*, 2006, 201(7):4201–4204.）

(3) 论文题目 “Molecular dynamics simulation of the (0 0 0 1)  $\alpha\text{-Al}_2\text{O}_3$  and  $\alpha\text{-Cr}_2\text{O}_3$  surfaces”（出自 Jizhong Sun, T. Stirner, A. Matthews. *Molecular dynamics simulation of the (0 0 0 1)  $\alpha\text{-Al}_2\text{O}_3$  and  $\alpha\text{-Cr}_2\text{O}_3$  surfaces*[J]. 2007, 601(5):1358-1364.）

点评：以上三篇文献论文题目实词分别为 11、10、9 个；题目均选用名词。概括精准，突出了论文的重要内容，见名知意。

## 三、摘要

1. 摘要是一片论文的总结，一般为 250 字左右。
2. 陈述论文研究的主要目的和范围，研究采用的方法，总结研究结果，给出研究得出的主要结论。

3. 不能出现论文中没有的信息和结论，不能引用参考文献，不能出现表格和图片，不能包含过多细节信息，要字斟句酌。

举例如下：

(1) 论文摘要 “Alumina and chromia are very important materials in the surface coatings industry, e.g. for corrosion protection and as catalyst supports. The type of defects and the associated formation energy in these materials are of direct relevance to the surface stability and reaction kinetics. In the present work, a modified Matsui potential is applied to calculate the native point defect energies in  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> based on the Mott–Littleton theory. Particular attention is paid to the convergence of the defect energies with the number of atoms surrounding the defect. The results show that the relative values of the defect formation energies are such that the Schottky energy is smaller than either of the Frenkel energies, which is in agreement with experimental data and recent results of first-principles calculations. The implications of these findings for diffusion mechanisms and the associated reaction kinetics are discussed briefly.” (出自 Sun J, Stirner T, Matthews A. Calculation of native defect energies in  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> using a modified Matsui potential[J]. Surface and Coatings Technology, 2006, 201(7):4201–4204.)

(2) 论文摘要 “A simple, rigid pair-potential model is applied to investigate the dynamics of the (0 0 0 1)  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> surfaces using the molecular dynamics technique. The simulations employ a two-stage equilibration process: in the first stage the simulation-cell size is determined via the constant-stress ensemble, and in the second stage the equilibration of the size-corrected simulation cell is continued in the canonical ensemble. The thermal expansion coefficients of bulk alumina and chromia are evaluated as a function of temperature. Furthermore, the surface relaxation and mean-square displacement of the atoms versus depth into the slab are calculated, and their behaviour in the surface region analysed in detail. The calculations show that even moderate temperatures (400 C) give rise to displacements of the atoms at the surface which are similar to the lattice mismatch between  $\alpha$ -alumina and chromia. This will help in the initial nucleation stage during thin film growth, and thus facilitate the deposition of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> on (0 0 0 1)  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> templates.” (出自 Jizhong Sun, T. Stirner, A. Matthews. Molecular dynamics simulation of the (0 0 0 1)  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> surfaces[J]. 2007, 601(5):1358-1364.)

(3) 论文摘要 “Although high-entropy alloys (HEAs) are attracting interest, the physical metallurgical mechanisms related to their properties have mostly not been clarified, and this limits wider industrial applications, in addition to the high alloy costs. We clarify the physical metallurgical reasons for the materials phenomena (sluggish diffusion and micro-twinning at cryogenic temperatures) and investigate the effect of individual elements on solid solution hardening for the equiatomic CoCrFeMnNi HEA based on atomistic simulations (Monte Carlo, molecular dynamics and molecular statics). A significant number of stable vacant lattice sites with

high migration energy barriers exists and is thought to cause the sluggish diffusion. We predict that the hexagonal close-packed (hcp) structure is more stable than the face-centered cubic (fcc) structure at 0 K, which we propose as the fundamental reason for the micro-twinning at cryogenic temperatures. The alloying effect on the critical resolved shear stress (CRSS) is well predicted by the atomistic simulation, used for a design of non-equiatom fcc HEAs with improved strength, and is experimentally verified. This study demonstrates the applicability of the proposed atomistic approach combined with a thermodynamic calculation technique to a computational design of advanced HEAs.”（出自 Choi W M , Jo Y H , Sohn S S , et al. Understanding the physical metallurgy of the CoCrFeMnNi high-entropy alloy: An atomistic simulation study[J]. 2018.）

点评：以上三篇文献论文摘要均控制在 250 词左右，均简明扼要的陈述了研究目的、实验方法并给出了主要实验结果，只看摘要便可知此篇文献论文的大部分分类容。

## 四、引言

1. 引言应该说明作者开展科研的原因，要简明扼要的陈述写作目的，研究方向的优点与不足、体现自己的研究领域和国内外现状、展现创新性。

2. 明确指出采用的研究方法，必要时应指出采用该特定研究方法的原因。

3. 陈述主要的研究结果并指出由研究结果得出的主要结论。

4. 参考文献要近些年或早期经典，并且水平要高，中心期刊以上。

举例如下：

(1) Alumina and chromia are very important materials in the surface coatings industry, e.g. for corrosion protection, catalyst supports, dielectric insulators, etc. The type of defects and the associated formation energy in these materials are of great importance for atomic transport and mechanical properties, and are of direct relevance to the surface stability and reaction kinetics. Within the constraints of charge neutrality and stoichiometry, only two types of native point defects are allowed in  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub>, i.e. Schottky and Frenkel defects. There are numerous theoretical studies on these intrinsic point defects in the corundum-type crystals, e.g. Al<sub>2</sub>O<sub>3</sub> (Refs. [1–4]), Cr<sub>2</sub>O<sub>3</sub> (Refs. [4–6]) and Fe<sub>2</sub>O<sub>3</sub> (Refs. [4,5,7]). Most of these studies employed the same empirical shell model [8] (albeit with different parameter sets) combined with the Mott–Littleton approximation [9], although Catlow et al. [2,5] and Lawrence [6] also carried out calculations with an interatomic potential from a modified form of the electron-gas approximation. Very recently, first-principles calculations have been performed for intrinsic defects in  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> [10]. However, there is still some controversy over the dominant defect type in  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>. Some calculations [2,3] indicate that oxygen Frenkel defects have a lower

formation energy than Schottky defects, while others [1,2,4,10] come to the opposite conclusion. As pointed out by Catlow et al. [2], this may in part be due to the difference in potential parameters used for describing the properties of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>. As mentioned above, to date the Mott – Littleton approximation has been the predominant method to carry out calculations of defect energies. In contrast to first-principles calculations, the main advantages of the Mott – Littleton method are its easy implementation and low computational cost. In general, it is thought that approximately 100 atoms around a defect are sufficient for a convergence of the Mott – Littleton calculations [2]. However, about 40 atoms or less were also used to calculate defect energies [1,4]. Hence, it is necessary to examine the convergence of the results when the Mott – Littleton method is used. In a previous paper [11] we developed a very simple potential from the model put forward by Matsui [12], which can describe the structure and lattice energy of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> very well. This “modified” Matsui model is very similar to shell models, except that in the latter a point charge is separated into a shell and a core. The shell is attached to the core by a spring and the overlap of shells results in a short-range repulsion. This modification leads to several additional parameters in the interaction potential, which requires at least the same number of experimental observables for their parameterisation [13]. In the present paper we will transfer this modified Matsui potential from  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> to  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> in order to calculate the native point defect energies for both crystals. The convergence of the calculations using the Mott – Littleton approximation will be tested, the predicted order of native defect energies in stoichiometric  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> presented, and the importance of the investigated lattice defects for reaction kinetics and diffusion mechanisms etc. discussed. (出自 Sun J , Stirner T , Matthews A . Calculation of native defect energies in  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> using a modified Matsui potential[J]. Surface and Coatings Technology, 2006, 201(7):4201–4204. )

(2) The properties of metal oxides are of considerable interest, e.g. for applications in the surface-coatings industry. Numerous static quantum-mechanical calculations and atomistic simulations have been carried out on surfaces of metal oxides. In contrast, relatively few surface-dynamics studies can be found in the literature. Recently, several dynamics studies (mostly using molecular dynamics simulations) have been performed, e.g. on premelting processes in Cr<sub>2</sub>O<sub>3</sub> [1], the (0 0 0 1) Cr<sub>2</sub>O<sub>3</sub> surface [2], the MgO surface [3], the CeO<sub>2</sub> surface [4,5], the  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> surface [6,7], the (0 1 1)CeO<sub>2</sub>/(0 0 0 1)Al<sub>2</sub>O<sub>3</sub> interface [8], and the (1 0 0), (1 1 0) and (1 1 1) NiO surfaces [9,10]. These studies have shown that the displacements of the atoms in the surface region are relatively large, which was also confirmed independently via low-energy electron diffraction measurements [11]. Large, short-lived displacements of the surface atoms may also be important for catalytic processes [8]. As a member of the corundum-type family,  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> is widely studied owing to its technological and fundamental scientific importance [12 – 15]. Our interest in the surface dynamics of  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> stems from recent findings that chromia can be used for the templated growth of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> thin films at drastically reduced substrate temperatures of

280 – 560 C [16,17]. Conventional techniques for the growth of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> films, such as chemical vapour deposition (CVD), require substrate temperatures of over 1000 C [18], which severely limits the range of practical applications. Andersson et al. [16] suggest that the surface mobility is large over the investigated temperature range (280 – 560 C) and that the high temperatures used for nonepitaxial  $\alpha$ -alumina deposition are primarily needed to promote initial grain nucleation. Surface mobility and migration barriers for a (0 0 0 1)  $\alpha$ -alumina surface were recently studied via an ab initio molecular dynamics technique by Rose et al. [19 – 21]. Using an ab initio periodic Hartree – Fock (PHF) method, we have recently investigated the structure and energy of low-index  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> surfaces, where we found that the  $\bar{1}10\bar{1}2g$  and {0 0 0 1}  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> planes are suitable candidates for the templated growth of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> thin films [15]. Although there is still some controversy over the termination of the (0 0 0 1)  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> surface [22], most studies provide evidence supporting the Cr-terminated surface [13,14,23,24]. Previous molecular dynamics (MD) simulation studies on the (0 0 0 1)  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> surface mainly focused on the pre-melting processes [1,2]. In Ref. [25], we presented the dynamics of the (0 0 0 1)  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> surface calculated with the canonical ensemble at 10 and 100 K, where we found the mean-square displacement (msd) of the atoms to vary non-monotonically as a function of depth into the slab. In the present paper, we will first revisit the (0 0 0 1)  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> surface in order to see if these non-monotonic variations persist at higher temperatures. We will then concentrate on the dynamics of the (0 0 0 1)  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> surface. (出自 Jizhong Sun, T. Stirner, A. Matthews. Molecular dynamics simulation of the (0 0 0 1)  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> surfaces[J]. 2007, 601(5):1358-1364.)

点评：以上两篇文献论文引言均说明了作者开展科研的原因，并要简明扼要的陈述写作目的，研究方向，体现了自己的研究领域和国内外现状，并展现了创新性。明确指出采用的研究方法，并指出了采用该特定研究方法的原因。陈述了主要的研究结果并指出由研究结果得出的主要结论。而且参考文献均为论文发表前五年内高水平文献。

## 五、实验

1. 实验这一章节目的是告诉读者，所使用的使用方法、技术手段而获得的结果是可靠的。

2. 需要确保足够细致地解释说明实验方法，提供尽可能多的细节，让论文阅读者可以凭此重复这些实验，必要时，要解释为什么采用这种实验方法。

3. 一般在论文中避免采用材料的商品名称，最好使用通用名或者化学名称。

4. 一般使用时间顺序描述实验方法，不过对于关系紧密的集中方法，放在

一起描述更好。

5. 实验章节通常有副标题，在使用时应查看欲投期刊上的类似论文，尽可能使副标题与结果部分出现的内容前后一致。

6. 撰写时，文字、图、表要相对独立，尤其应该避免重复。

举例如下：

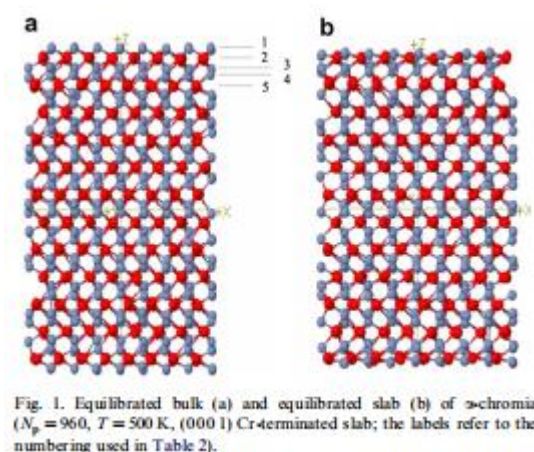
(1) In our previous work [25], we developed an empirical model for  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> in which the atomic interactions are described by a Buckingham potential plus a Coulomb term. In Ref. [26], we transferred this potential to  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> which has the same corundum-type structure and similar lattice constants to  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>. For both material systems it was found that the repulsive interactions between cations are negligible and the resulting potential takes the form

$$V(r_{ij}) = \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} - \frac{C_{OO}}{r_{ij}^6} + A_{OO} \exp\left(-\frac{r_{ij}}{\rho_{OO}}\right) + A_{MO} \exp\left(-\frac{r_{ij}}{\rho_{MO}}\right)$$

where O represents oxygen and M = Al or Cr. The potential parameters for  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> are  $A_{AlO} = 3411.118$  eV,  $q_{AlO} = 0.244549$  Å° [25], and for  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> they are  $A_{CrO} = 2362.905$  eV,  $q_{CrO} = 0.270628$  Å° , with  $A_{OO} = 91.55955$  eV,  $q_{OO} = 0.547148$  Å° and  $COO = 32.32$  eV Å°<sup>6</sup> [26]. Cations and anions take their full formal charges. As was shown in Refs. [25,26], this empirical model is able to describe the structural properties of alumina and chromia very well. The calculated lattice constants for  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> are  $a_0 = 4.773$  Å° and  $c_0 = 12.990$  Å° (experiment  $a_0 = 4.760$  Å° and  $c_0 = 12.993$  Å° [27]), and for  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> they are  $a_0 = 4.987$  Å° and  $c_0 = 13.558$  Å° (experiment  $a_0 = 4.951$  Å° and  $c_0 = 13.556$  Å° [28]). In contrast to the shell model [29], the present model ignores polarization effects. Including these effects makes not only the parameterisation more difficult but also the MD equilibration process much more time-consuming. In this context, we note that Barrera et al. [1] have shown that polarization effects are negligible in some melting processes. However, these effects are also reflected in the high-frequency dielectric constant  $\epsilon_1$  and become more important for large differences between  $\epsilon_1$  and unity. Since rigid models, whose potential parameters are usually obtained from fitting bulk properties, cannot self-consistently adjust to a new environment, they may not be adequate to describe surfaces and defects [30]. Whether a rigid model can be applied to the surface depends on how different the charges that the ions carry at the surface are from the bulk. Recently, ab initio Hartree–Fock calculations [31] showed that Cr carries only slightly less charge at the surface (2.13  $e_j$ ) compared to the bulk (2.31  $e_j$ ), with a concomitant decrease of the nearest Cr–O separation from 1.99 Å° in the bulk to 1.80 Å° at the surface. Thus, we anticipate that the error introduced by a rigid model is relatively small. In the present work, the surface relaxation at zero temperature is carried out by a static calculation using the computer code METADISE [32]. For non-zero temperatures, we employ the MD computer code DL\_POLY (Version 2.15) [33] with a slab model to calculate the

surface dynamics. Here we choose an orthorhombic simulation cell (with periodic boundary conditions) of 960 particles with cell faces  $\delta 1\ 12\ 0\text{\AA}$ ,  $\delta 1\ 01\ 0\text{\AA}$  and  $(0\ 0\ 0\ 1)$ , measuring  $V = X \cdot Y \cdot Z = 19.949 \cdot 17.276 \cdot 27.116\ \text{\AA}^3$  at zero temperature. Since the cell expands with temperature, it is necessary to find the new dimension of the simulation cell for a specific temperature before the surface relaxation can be studied. Consequently, it is important to employ appropriate thermodynamic ensembles to conduct the equilibration procedure. We equilibrate the bulk system as follows: first, we choose the constant-stress ensemble (Berendsen thermostat and barostat [33]) to find the cell dimension at a specific temperature; we relax the simulation cell for at least 80 ps with a time step of 0.4 fs; we then replace the constant-stress ensemble with the canonical ensemble (Evans thermostat [33]) and relax the system with the new dimension again for at least 64 ps, and finally perform a production run of 32 ps. For the calculations pertaining to surfaces, a slab (which is cut directly from the equilibrated bulk) is equilibrated further for at least 64 ps, and then a production run of 32 ps is performed with data output every 4 fs. Fig. 1 shows snapshots of the equilibrated bulk (a) and equilibrated slab (b) of the chromia crystal (at  $T = 500\ \text{K}$ ) employed in the present work. The meansquare displacement in the z-direction for the  $j$ th ion is defined as  $\text{msd}_{zj} = \frac{1}{N} \sum_{i=1}^N (z_{ij} - z_j)^2$  with  $z_j = \frac{1}{N} \sum_{i=1}^N z_{ij}$ , where  $i$  denotes the  $i$ th output data and  $N$  represents the total number of data outputs (in our calculations  $N = 8000$ ); the other components of  $\text{msd}$  are defined in the same way. Finally, the  $\text{msd}_j$  values are averaged over each plane (the assignment of atoms to planes is still meaningful over the temperature range investigated in the present study). We have checked the statistical fluctuations of the mean-square displacements and for all cases these are smaller than 4% (8%) for atoms in the bulk (surface).

(出自 Jizhong Sun, T. Stirner, A. Matthews. Molecular dynamics simulation of the  $(0\ 0\ 0\ 1)$   $\alpha$ - $\text{Al}_2\text{O}_3$  and  $\alpha$ - $\text{Cr}_2\text{O}_3$  surfaces[J]. 2007, 601(5):1358-1364.)



点评：此篇文献的实验章节，方法细节足够细致，包括建模模拟步骤，单位原子电荷键角、模拟方程等细节，并提供模拟结果。使我们可以轻易复制此模拟方法在自己的计算机上，并且可以对比文献结论，验证自己计算是否正确，以便改正。



## 六、结果与讨论

1. 结果与讨论部分是整篇论文的归节点，而不是某一局部问题或某一分支问题的结论，也不是正文各章节小结的简单重复。
2. 应当体现作者更广和更深层的认识和思考。
3. 陈述主要结果，解释主要结果与问题假设的关系。
4. 陈述主要结论，陈述研究成果的理论意义和实际价值。
5. 指出研究的局限性和未来的研究方向。
6. 讨论要分清主次，既要有深度又要有广度。
7. 讨论要措辞严谨，逻辑紧密。

举例如下：

### (1) 1. Thermal expansion coefficients

Before focusing on the surface properties of (0 0 0 1) a-Al<sub>2</sub>O<sub>3</sub> and a-Cr<sub>2</sub>O<sub>3</sub>, we briefly discuss the thermal expansion of bulk a-alumina and chromia. The thermal expansion coefficient  $\beta$ , defined by is used to express the volume change of a substance due to a temperature change [34]. Strictly speaking, the simulation cell for the system considered here is not exactly orthorhombic any more at non-zero temperatures, but the deformation is negligible at low to intermediate temperatures. As a first approximation, we assume that the volume depends linearly on temperature. Consequently, the new cell volume can be calculated by  $(X + DX) \cdot (Y + DY) \cdot (Z + DZ)$ , and the thermal expansion coefficient  $\beta$  can be approximated by

$$\beta = \frac{1}{V} \left. \frac{\Delta V}{\Delta T} \right|_p$$

The calculated thermal expansion coefficients for a-Al<sub>2</sub>O<sub>3</sub> and a-Cr<sub>2</sub>O<sub>3</sub> are summarized in Table 1, together with the available experimental data taken from Refs. [35,36]. As can be seen, the present model is able to reproduce the thermal expansion coefficients for a-alumina reasonably well, while the corresponding values for a-chromia are significantly overestimated. This is hardly surprising, since the parameterisation was carried out for a-alumina and then transferred to a-chromia, and the experimental thermal expansion coefficients did not enter the cost function during the parameterisation procedure. Nevertheless, as far as the accuracy of the dynamical data are concerned, we note that the error introduced by this uncertainty in the chromia potential is significantly smaller than the statistical fluctuations of the mean-square displacements of the atoms. In contrast, we have found that it is important to take the thermal expansion of the system into account (via the equilibration procedure described in Section 2 above) in order to obtain accurate values of the meansquare displacements.

Table 1  
Calculated and experimental thermal expansion coefficients (in  $10^{-6} \text{ K}^{-1}$ )  
for  $\alpha\text{-Al}_2\text{O}_3$  and  $\alpha\text{-Cr}_2\text{O}_3$  at different temperatures  $T$

$T$ (K)	Calculated $\alpha\text{-Al}_2\text{O}_3$	Experimental Ref. [35]	Calculated $\alpha\text{-Cr}_2\text{O}_3$	Experimental Ref. [36]
100	22.8	–	21.6	–
300	22.6	23.0	25.6	16.0
500	24.5	24.5	27.1	18.5
700	28.9	25.5	25.3	19.5

## 2. Surface relaxation

We now apply the present model to investigate the relaxation of the (0 0 0 1)  $\alpha\text{-Cr}_2\text{O}_3$  surface. The obtained percentage changes in the interplanar spacings after full relaxation are summarised in Table 2. As can be seen, the present calculations agree reasonably well with the experimental results of Rohr et al. [23] using low-energy electron diffraction (LEED). Our calculations are also consistent with previous theoretical works in that all of these studies predict a large surface relaxation, i.e. the top Cr layer moves inward quite substantially while the second layer relaxes relatively little. However, the present model predicts a (0 0 0 1)  $\alpha\text{-Cr}_2\text{O}_3$  surface energy of  $0.9 \text{ J m}^{-2}$ , which is considerably lower compared to other studies; e.g. Rohrbach et al. [14] predict a value of  $1.4 \text{ J m}^{-2}$  using density functional theory, while Rowley et al. [37] obtained  $4.8 \text{ J m}^{-2}$  with an aspherical ion model (AIM).ace relaxation.

## 3. Surface dynamics

Before discussing the dynamics of the (0 0 0 1)  $\alpha\text{-Al}_2\text{O}_3$  and  $\alpha\text{-Cr}_2\text{O}_3$  surfaces, we briefly describe the calculated average bulk mean-square displacement (msd) values. The latter are summarised in Table 3 together with the experimental data of Lewis et al. [27] and the MD simulation results of Baudin et al. [6]. As can be seen, our calculated msd values are in reasonable agreement with the available experimental data for  $\alpha\text{-Al}_2\text{O}_3$ . All of these studies predict that the msdz values are larger than the corresponding msdxy values, and that the msd values for

Table 2  
Percentage changes in interplanar spacings (see Fig. 1) at the surface of a fully relaxed (0001) slab of  $\alpha\text{-Cr}_2\text{O}_3$

Method	$d_{12}$	$d_{23}$	$d_{34}$	$d_{45}$	Reference
Exp (LEED)	–60	–3	–21	6	[23]
AIM	–40	6	–30	11	[37]
Shell	–59	13	–54	31	[38]
GGA + $U$	–60	12	–44	9	[14]
PHF	–49	3	–47	11	[15]
Static	–62	0	–51	23	This work

**Table 3**  
Average mean-square displacement of atoms (in  $10^{-3} \text{ \AA}^2$ ) for bulk  $\alpha\text{-Al}_2\text{O}_3$  and  $\alpha\text{-Cr}_2\text{O}_3$  at various temperatures ( $M = \text{Al, Cr}$ )

$T$ (K)	$\overline{\text{msd}}_{xy}^M$	$\overline{\text{msd}}_z^M$	$\overline{\text{msd}}_{xy}^O$	$\overline{\text{msd}}_z^O$	Reference
$\alpha\text{-Al}_2\text{O}_3$					
300	2.8	3.2	3.3	3.7	Exp [27]
300	1.6	1.8	2.3	2.9	MD [6]
300	2.2	2.6	2.3	2.9	This work
500	3.8	4.5	3.9	5.0	This work
$\alpha\text{-Cr}_2\text{O}_3$					
100	0.8	1.0	0.8	1.2	This work
300	2.4	3.2	2.6	3.5	This work
500	4.5	5.3	4.7	5.9	This work
700	6.2	8.2	6.7	8.8	This work

oxygen ions are slightly larger than those for metal ions. However, it has to be noted that the calculations are not compatible with the results of the X-ray diffraction study of Ishizawa et al. [39] on  $\alpha\text{-Al}_2\text{O}_3$  who predict that  $\text{msd}_{xy} > \text{msd}_z$  with relatively large  $\text{msd}_{xy}$  values (of  $5.1 \cdot 10^3 \text{ \AA}^2$  at room temperature). Considering the fact that an aluminium atom is about 1.5 times heavier than an oxygen atom and a chromium atom is more than 3 times heavier than an oxygen atom, we do not observe any significant mass dependence of the msd values. However, as can be seen from Table 3 and the results presented in Ref. [25], the msd values for  $\alpha\text{-Al}_2\text{O}_3$  and  $\alpha\text{-Cr}_2\text{O}_3$  are almost directly proportional to temperature.

Fig. 2 shows the normalised msd values of Al and O ions (i.e. divided by the corresponding average bulk values) for the (0 0 0 1)  $\alpha\text{-Al}_2\text{O}_3$  surface as a function of depth  $z$  into the slab at temperatures of 300 and 500 K. As can be seen, the main features observed in Ref. [25] at 10 and 100 K also appear at these higher temperatures: namely, the Al msd values vary highly non-monotonically as a function of  $z$  in the surface region; the outermost Al layer (having bulk alumina on one side and vacuum on the other side) exhibits the largest msd value, while the outermost O layer (sandwiched between the top two Al layers) has a much smaller msd value than the second O layer. Our normalised  $\text{msd}_z$  values for Al and O at the surface are smaller than those obtained by Baudin et al. [6] but are in good agreement with the quasiharmonic lattice dynamics results of Marmier and Finnis [7].

Next, we focus on the dynamics of the (0 0 0 1)  $\text{Cr}_2\text{O}_3$  surface. The normalised Cr and O msd values for this surface are shown in Figs. 3 and 4, respectively, at temperatures of 100, 300, 500 and 700 K. As can be seen, the dynamics of the (0 0 0 1)  $\alpha\text{-Cr}_2\text{O}_3$  surface region displays similar features to its  $\alpha\text{-Al}_2\text{O}_3$  counterpart: the Cr  $\text{msd}_z$  values of the outermost six layers exhibit highly non-monotonic variations as a function of depth  $z$  into slab; inside the sixth Cr layer the Cr msds are essentially equal to the corresponding bulk values. As expected, the Cr ions in the outermost surface layer exhibit the largest displacements since there are no neighbouring atoms on one side

of the layer to constrain their movements. In contrast, it is somewhat unexpected that the Cr ions in the third and fifth Cr layers have similar  $\text{msdz}$  values, while the Cr ions in the fourth Cr layer have very low  $\text{msdz}$  values (even slightly smaller than the corresponding bulk values). The latter can be attributed to the relatively large expansion of the fourth interplanar spacing  $d_{45}$  (see Table 2). Overall, the  $\text{msd}$  versus  $z$  curves for Cr at the  $(0\ 0\ 0\ 1)$   $\alpha\text{-Cr}_2\text{O}_3$  surface have a very similar shape over the whole investigated temperature range. Similarly, both components of the  $\text{O}$   $\text{msd}$  versus  $z$  curves for  $(0\ 0\ 0\ 1)$   $\alpha\text{-Cr}_2\text{O}_3$  (shown in Fig. 4) display nearly the same behaviour over this temperature range (the  $\text{msds}$  for the higher temperatures converge to their bulk value slightly deeper in the slab). The paramount feature of these curves is that the  $\text{msd}$  value of the oxygen ions in the second O layer is largest, while the  $\text{msds}$  in the outermost oxygen layer are significantly reduced. This arises from the large relaxation of the outermost Cr ions, which essentially sink into the first oxygen layer (see  $d_{12}$  in Table 2). Since the O ions are close packed on the  $(0\ 0\ 0\ 1)$  oxygen planes, the movement of these ions in this plane is quite restricted and therefore the  $\text{msd}_{xy}$  values are smaller than the  $\text{msdz}$  values. As pointed out above, the first O layer is sandwiched between the first and second Cr layers, the second O layer is sandwiched between the third and fourth Cr layers, and the third O layer is sandwiched between the fifth and sixth Cr layers. We notice from Fig. 3 that the  $\text{msdz}$  value of the Cr ions in the fourth Cr layer is relatively low, while the other Cr surface layers have relatively large  $\text{msdz}$  values. Similarly, from Fig. 4 it can be seen that only O layer number two has a significantly enhanced  $\text{msd}$  value, while the other surface O layers have moderate  $\text{msd}$  values. We attribute this behaviour to the overall dynamical balance of the system, which favours the stabilization of the surface. For instance, if the  $\text{msd}$  values of O ions in a certain layer are high, then the metal ions in the neighbouring layers have relatively low average  $\text{msd}$  values. Figs. 3 and 4 show that the maximum value of the normalised  $\text{msdz}$  for  $(0\ 0\ 0\ 1)$   $\alpha\text{-Cr}_2\text{O}_3$  is around 1.8. Compared to surface and bulk root mean-square displacement ratio data of metals compiled by Somorjai [40], this value is relatively low. For instance, the ratio of the  $\text{msdz}$  value for the metallic  $(110)$  Cr surface to bulk Cr is 3.2. As Somorjai [40] pointed out, the mean-square displacement of surface atoms is very sensitive to changes in the number and type of neighbouring atoms. The coupling strength between neighbouring atoms also affects the phonon density of states. A recent layer-by-layer analysis of the local phonon density of states for  $(100)$  and  $(110)$  NiO [10] seems to corroborate the present results. Finally, we have evaluated the mean displacement of the Al and Cr surface atoms in the basal plane. We have found that, at a temperature of 400 C, the combined mean displacement  $\bar{\text{md}}_{\text{Al } xy} = 0.09\text{ \AA}$  and  $\bar{\text{md}}_{\text{Cr } xy} = 0.09\text{ \AA}$  is similar to the difference in

the lattice constants  $a_0$  between  $\alpha$ -alumina and  $\alpha$ -chromia ( $\Delta a_0 = 0.19\text{ \AA}$ ). This will help in the initial nucleation stage during thin film growth and aid the formation of small islands. We also believe that the mean-square displacements are intimately related to surface mobility, i.e. the

larger the msd values the larger the surface mobilities. Incidentally, such a temperature of 400 C is also consistent with the experiments of Andersson et al. [16,17] who employed substrate temperatures of 280 – 560 C for the successful overgrowth of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> on  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> templates. (出自 Jizhong Sun, T. Stirner, A. Matthews. Molecular dynamics simulation of the (0 0 0 1)  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> surfaces[J]. 2007, 601(5):1358-1364.)

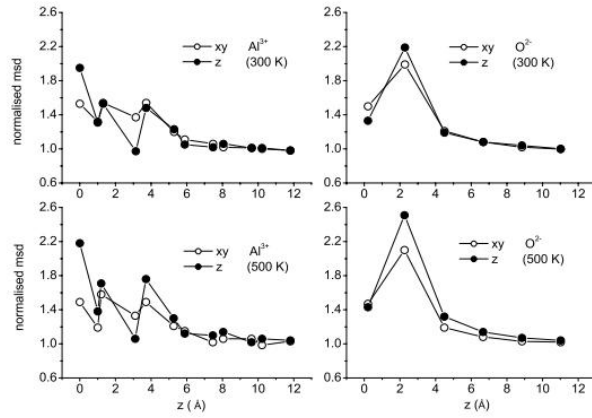


Fig. 2. Normalised mean-square displacements of oxygen and aluminium ions in a slab of (0001)  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> as a function of depth  $z$  into the slab ( $T = 300$  and 500 K). The msd values are divided by the corresponding average bulk msd values (see Table 3). The figure shows only one half of the slab; the curves are essentially symmetrical with respect to the centre of the slab.

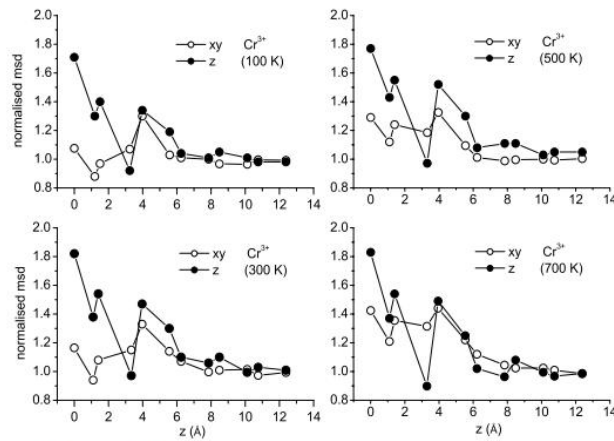


Fig. 3. Normalised mean-square displacements of chromium ions in a slab of (0001)  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> as a function of depth  $z$  into the slab ( $T = 100, 300, 500$  and 700 K). The msd values are divided by the corresponding average bulk msd values (see Table 3). The figure shows only one half of the slab; the curves are essentially symmetrical with respect to the centre of the slab.

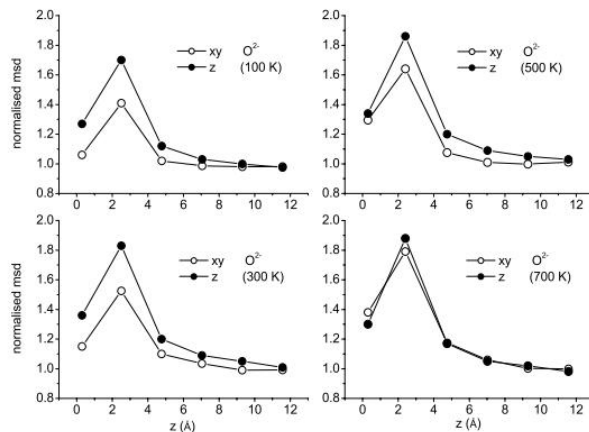


Fig. 4. Same as Fig. 3, except that the msd values are for oxygen ions.

点评：本篇文献的结果与讨论部分，分别从热膨胀系数、晶体表面弛豫与表面动力学三个方面层层推进，陈述了均方位移与表面迁移率的密切关系，均方位移越大，表面迁移率越大。在文字部分，没有重复描述实验部分已给出的实验细节。并且图表简洁清晰，让读者直接看到了不同参数对实验结果的影响。

## 七、结论

1. 结论是为读者提供整篇文献的一个总结，指出解决了什么问题。
2. 写结论时要把实验结果数据写的具体详细，把文章得到的结果结论都要阐述详尽。
3. 不要重复描述实验部分给出的实验细节。
3. 注意与摘要的区别：摘要是为读者提供文章的大题内容和文章的结构。摘要在论述过程中结果可以笼统些，不需要把实验数据信息写的那么具体。

举例如下：

(1) Molecular dynamics simulations of the (0 0 0 1)  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> surfaces have been carried out. Over the investigated temperature range the magnitude of the mean-square displacement values for the atoms in the bulk was found to be nearly linearly dependent on temperature, while the normalised mean-square displacements at the surface of the slabs are almost independent of temperature. The calculations also revealed that the mean-square displacement values of the anions are slightly larger than those of the cations, but essentially independent of ionic mass. The msdz values of the cations were found to vary non-monotonically as a function of depth  $z$  into the slab, with a maximum ratio of msdz at the surface to bulk of about 2.1 for Al and 1.8 for Cr. The O ions in the outermost oxygen layer were found to have much smaller msd values than in the second oxygen layer. Overall, the dynamics of both the (0 0 0 1)  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> surfaces show a very similar behaviour, which should favour the templated growth of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> on the (0 0 0 1)  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> surface. One of the problems for the templated growth of  $\alpha$ -alumina on chromia is the large strain due to the lattice mismatch between the two materials. A moderate increase in temperature to 400 C gives rise to an increase in the mean displacements of the atoms at the surface which is similar to the lattice mismatch between  $\alpha$ -alumina and chromia. This will help in the initial nucleation stage and the formation of small islands, and thus facilitate the growth of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> on (0 0 0 1)  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> templates. (出自 Jizhong

Sun, T. Stirner, A. Matthews. Molecular dynamics simulation of the (0 0 0 1)  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> surfaces[J]. 2007, 601(5):1358-1364.)

(2) Using a modified Matsui potential and the Mott - Littleton approximation we have calculated the formation energies of point defects in  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub>. The convergence of the calculated point defect energies was examined as a function of the system size. It was found that more than approximately 500 ions in region I are required for a convergence of the calculated vacancy and interstitial energies. The defect energy sequence of ESchbEMFbEOF, obtained by the present model for both  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub>, is consistent with recent firstprinciples calculations. As was pointed out previously [4], Schottky quintets seem to be the dominant intrinsic point defects in  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub>. Consequently, the metal cations are believed to be the more mobile species and are expected to diffuse via a vacancy mechanism. However, since the intrinsic defect energies in  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> are relatively large, the point defect chemistry in these materials will be controlled by small concentrations of aliovalent impurities [3]. Hence, cation vacancy compensation will dominate after tetravalent ions enter as cation substitutionals [2]. Recent advances in computing technology have enabled ab initio calculations of the stability and diffusion of oxygen vacancies in  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> [18,19]. Energy barriers for O-vacancy diffusion were found to be correlated to the Madelung potential at the saddle point for ionic compounds. (出自 Sun J, Stirner T, Matthews A. Calculation of native defect energies in  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> using a modified Matsui potential[J]. Surface and Coatings Technology, 2006, 201(7):4201-4204.)

点评：以上两篇文献论文结论，均对所做实验给出了准确的总体描述，实验数据清晰明了，指出了解决的问题，读者读完后能够了解此文献的研究意义。

## 八、致谢

1. 致谢内容要包含感谢资金的来源，感谢帮助自己完成论文的重要人物。
2. 致谢态度要端正，措辞要恰如其分。

举例如下：

(1) This work is supported by the EPSRC (UK) under grant GR/S05632/01. J. Z. S gratefully acknowledges Prof. J. D. Gale for providing him with the General Utility Lattice Program (GULP) code. (出自 Sun J, Stirner T, Matthews A. Calculation of native defect energies in  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and

$\alpha$ -Cr<sub>2</sub>O<sub>3</sub> using a modified Matsui potential[J]. Surface and Coatings Technology, 2006, 201(7):4201–4204. )

(2) This work is supported by the EPSRC (UK) under Grant GR/S05632/01. The authors are indebted to Prof. J.H. Harding for helpful discussions. Dr. D.J. Cooke is thanked for help with the METADISE computer program.(出自 Jizhong Sun, T. Stirner, A. Matthews. Molecular dynamics simulation of the (0 0 0 1)  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> surfaces[J]. 2007, 601(5):1358-1364.)

点评：以上两篇文献论文的致谢部分内容简洁明了，均感谢了资金来源，与完成论文提供帮助的重要人物。

## 九、参考文献

1. 在保证文献引用的必要性、充分性和代表性的前提下，学术期刊论文参考文献引用数量和范围应当尽量全面。

2. 引用文献要具有权威性、以期刊型文献和专著型文献为主，结合引用经典文献和新颖文献，辩证引用中外文献。

3. 研究者还应当有意识的注意论文中参考文献的引用位置，并做到文献编辑格式的规范统一。

4. 选择的参考文献在数目上要多一些，覆盖范围要全面。

5. 各类期刊对参考文献要求不一样，常用格式有三种：著者姓名-出版年；引用次序；字母-数字。

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点评：以上两篇文献论文的参考文献部分编辑格式规范统一，且引用全面。

## 十、回复审稿人意见

1. 注意态度诚恳，正确理解审稿人的意见。
2. 依次对每个意见进行逐条回复，耐心解释，必要时注明文献来源。

3. 尽量满足意见中需要补充的实验，并对于满足不了的意见不要回避，说明理由。

4. 回复时间要有时效性，体现对审稿人的尊重，并为及时发文奠定基础。

## 十一、最后

由衷感谢王老师悉心讲授，本课程是学生研究生以来最实用的一门课程，通过系统学习，让我对如何写作英语论文有了细致了解，以至于在需要写论文时知道如何下笔。老师作业形式新颖，通过完成作业，更加深了对论文框架的理解。此作业，学生会一直留存。最后，由衷感谢王老师的讲授，谢谢！