A SURFACE DEFINITION METHOD FOR AN INTERFACIAL ENERGY DATABASE

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ABSTRACT

Agreeing on a method to identify interfaces is a desirable step in order to build a database of interfacial energy. So far, the expression Sigma X Interface has been used to identify interfaces. Unfortunately, this conventional method cannot express arbitrary interface geometries. In the present work, we review interface geometries and propose a systematic Orientation Method based purely on geometrical considerations that can express arbitrary twists and slipping of interfaces.

Keywords: Sigma X, Interface, Database, Geometry

1 INTRODUCTION

A systematic Interface identification method is a desirable step in order to build a database of interfacial energy. Kunio Takahashi, (2001) has pointed out the significance of a database and have a series of procedures for calculation and experiments (Yamaguchi, Takahashi & Onzawa, 2000; Takahashi, Nara, Yamaguchi & Onzawa, 1999); however they have not suggested a method to identify interfaces. So far the expression *Sigma X Interface* (Ranganathan, 1966), has been used when referring to interfaces composed of a pair of surfaces / grain boundaries. However this has some drawbacks:
First, the expression *Sigma X Interface* cannot express arbitrary slippings. Second, it cannot express arbitrary pairs of interfaces made of different materials (Ranganathan, 1966), for example a BCC-FCC interface. Third, *Sigma X Interface* in spite of having a simple geometric interpretation is an ill-defined (Romeu, 2003) discontinuous (Romeu, 1999) function.

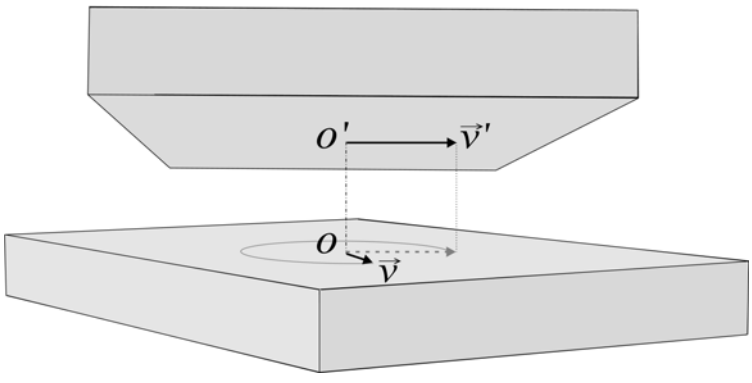

Figure 1. A generic twisted interface

Any single type grain boundary or interface (for example FCC 100 – FCC 100) can be associated to a *Coincidence Site Lattice (CSL)*. The relationship between an arbitrary *CSL* (characterized by the number Sigma X) and a given twist angle (miss-orientation) between a given pair of same-type surface planes was fully given by Ranganathan in 1966 (Ranganathan, 1966), for cubic systems.

The fact that interfaces with characteristic *Coincidence Site Lattices* should exhibit special characteristics was realized early on by Kronberg & Wilson (1949). This made of *Sigma X* an attractive choice for *labeling* interfaces. The underlying physical model could be used to predict properties. However, we know that the *CSL* model has some limitations and we cannot rely so much as we would like on it to predict properties of interfaces. Having pointed out the limitations of *Sigma* X in the following chapters we will introduce a simple rule of thumb that can label any type of interface geometry.

2 A DEFINITION METHOD

In order to identify interfaces we will follow a practical approach based on orientating surfaces. As we will show through a close-packet case example, orientating general case surface in a systematic way requires not only considering inner layers of atoms but also a symmetry-breaking scheme, albeit arbitrary. In the following section we will introduce this scheme and finally we will provide some examples of orientated surfaces.

2.1 Orientating surfaces

To orientate a surface it suffices an *Origin Point* and a *Direction*. In order to characterize interfaces under a given rotation or displacement it is first necessary to define a standard way to relatively orientate the pair of surfaces that form an interface. One way to do this is to define a point (a reference point *o*) and a direction (an orientation vector $\vec{v}$) for each surface. An example is shown in Figure 1 from a recent computer graphic representation.

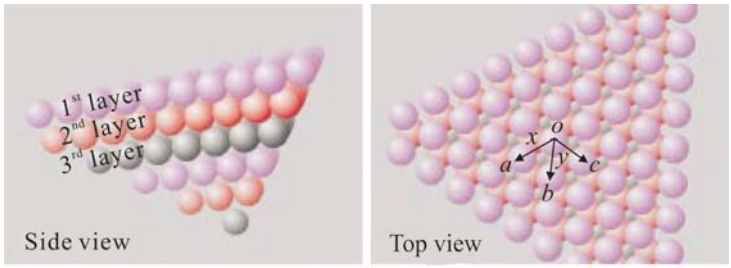

Figure 2. Top and side view of a FCC 111 Surface

2.2 Desired characteristics

We are looking for a method to systematically orientate surfaces, that is, a way to define an origin point *o* and a $\vec{v}$ orientating vector for each given surface. One natural choice for an origin point *o* is the center of one of the atoms in the surface. An example is shown in Figure 2. A natural choice for an orientating vector $\vec{v}$ is the difference vector between *o* and any of its neighboring atoms, for example, $\overrightarrow{oa}$, $\overrightarrow{ob}$, *and* $\overrightarrow{oc}$.

Lets take a FCC 111 surface. An example is shown in Figure 2. Note that once *o* is fixed there are 6 possible $\vec{v}$ choices. Each atom in the surface has 6 neighbors. Vectors $\overrightarrow{oa}$, $\overrightarrow{ob}$, *and* $\overrightarrow{oc}$ are 3 different valid orientation alternatives. Note that $\overrightarrow{oa}$, *and* $\overrightarrow{oc}$ directions are interchangeable, (and thus equivalent), but are not interchangeable with $\overrightarrow{ob}$ due to the arrangement of the inner layers. This is because if we choose $\overrightarrow{oa}$ as an orientating vector, we can see that in projecting the surface onto a plane (Figure 2, top view), departing from the origin point, the *1st* atom we encounter in the *2nd* layer is positioned to the right

(in the figure marked with an *x*). Had $\overrightarrow{ob}$ been selected , it would have been located to the left (*y* atom), hence, the need to define a general way to discriminate such ambiguities. We can deal with this problem through the concept of *Extended Unit Cell*.

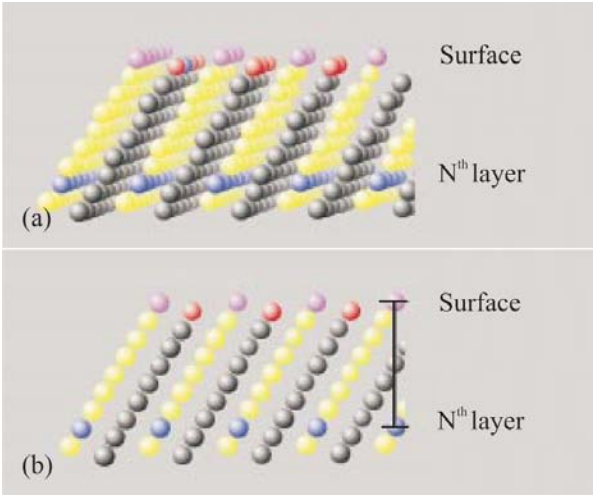

Figure 3. Layers and periodicity of a FCC 123

2.3 Layers and periodicity of a surface

When considering inner layers we can see by inspection that any surface can be regarded as being formed by a series of stacks of atoms parallel to the surface plane (such as in close-packed stacking ABCABC...), These parallel stacks are separated by a constant inter-planar distance. Their periodicity depends on the plane (defined by a Miller direction *h k l*) and on the crystal's lattice type. For example, a FCC 111 has a periodicity of 3, a FCC 211 one of 6, while a FCC 123 one of 14.

2.4 The Extended Unit Cell concept

Be it a FCC, BCC, or a diamond structure, we define the *Extended Unit Cell* (EUC) as the minimum perimeter base unit cell, whose base's vertexes each coincide with an atom of the surface we are concerned with, the upper basal plane being contained in the surface plane, and the bottom base being coincident with the closest N^{th} periodic layer from the surface. In other words, the Extended Unit Cell is just a non-primitive unit cell with the particularity that it takes into account the periodicity of the crystal from a surface dependent point of view. An example is shown in Figure 4. The principles that apply in the definition of the classic (West, 1999) Unit Cell also apply.

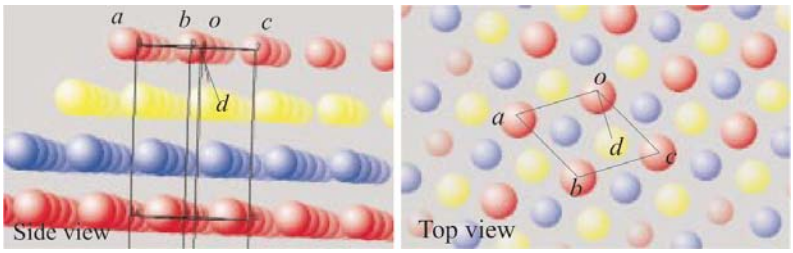

Figure 4. Side and Top view of an Extended Unit Cell for a FCC 111

3 AN ORIENTATION METHOD

The method we are looking for should have the following characteristics:

- Discriminates between left and right in order to avoid ambiguities such as the FCC 111 case.
- Must be unique: one surface, one orientation result.

Consequently, the method we propose is based on projecting the *Extended Unit Cell* into a plane parallel to the surface we are interested in, and choosing as an orientating vector one of the sides of the base of the *Extended Unit Cell*.

Note that this method is not strictly unique in a mathematical sense. However, by inspection we can see that it is unique for the crystal space we are concerned with here. Undetermined cases, such as the BCC 100 for instance, produce four side-vector orientation candidates, which incidentally are equivalent directions.

In mathematical form:

Origin Point = the center of any given atom of a surface.

Orientation Vector = the normalized side-vector, *(sv)* whose cross-product with normalized vector (*dv)* is Maximum for $v = a,b,c,o$, ie

Table 1. Orientating Criteria

$$Orientation\ Vector = \overrightarrow{sv}\Big|_{MAX\ \overrightarrow{sv}\times\overrightarrow{dv}}$$

for $(\overrightarrow{sv},\overrightarrow{dv}) = (\overrightarrow{oa},\overrightarrow{od}),(\overrightarrow{ab},\overrightarrow{ad}),(\overrightarrow{bc},\overrightarrow{bd}),(\overrightarrow{co},\overrightarrow{cd})$

where all vectors are normalized,

being *d* the coords of the Extended Unit Cell's *2 nd* layer atom

Examples of the proposed criteria are shown in Figures 5 to 7.

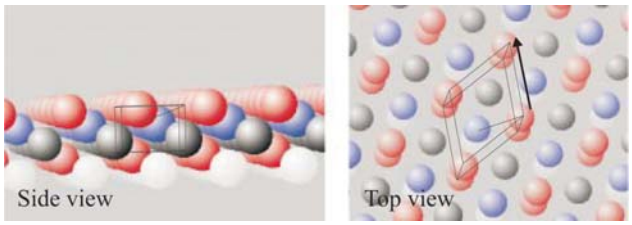

Figure 5. Side and top view of EUC and orientation for a FCC100 surface

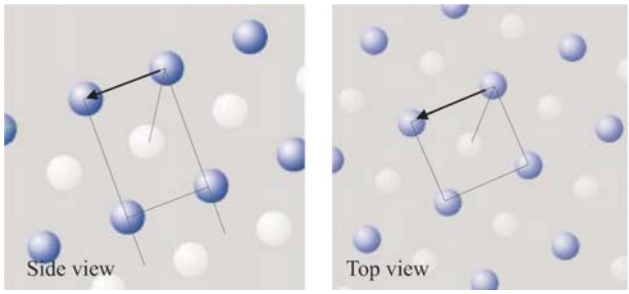

Figure 6. Side and top view of EUC and orientation for a BCC 111 surface

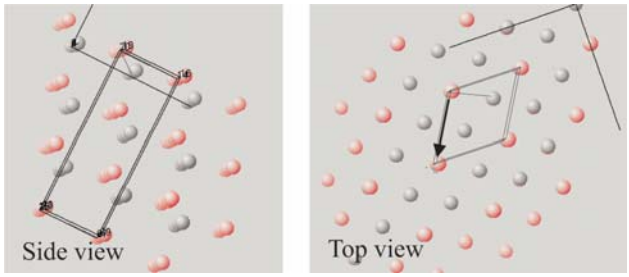

Figure 7. Side and top view of EUC and orientation for a Silicon / Diamond surface

4 CONCLUSION AND EXAMPLE

A geometric rule-of-thumb for orientating surfaces, and thus interfaces / bi-crystals, has been presented here. We hope that this scheme is useful in the standardization of physical measurements of interfaces. The rule we propose is based on the concept of *Extended Unit Cell*: A non-primitive cell linked to the surface plane (hkl) which might be interpreted as a primitive cell from a surface point of view. Following we introduce a practical example.

4.1 Database Example

Using the *Extended Unit Cell* method and setting one of the surfaces as a reference surface, a typical database entry looks like this

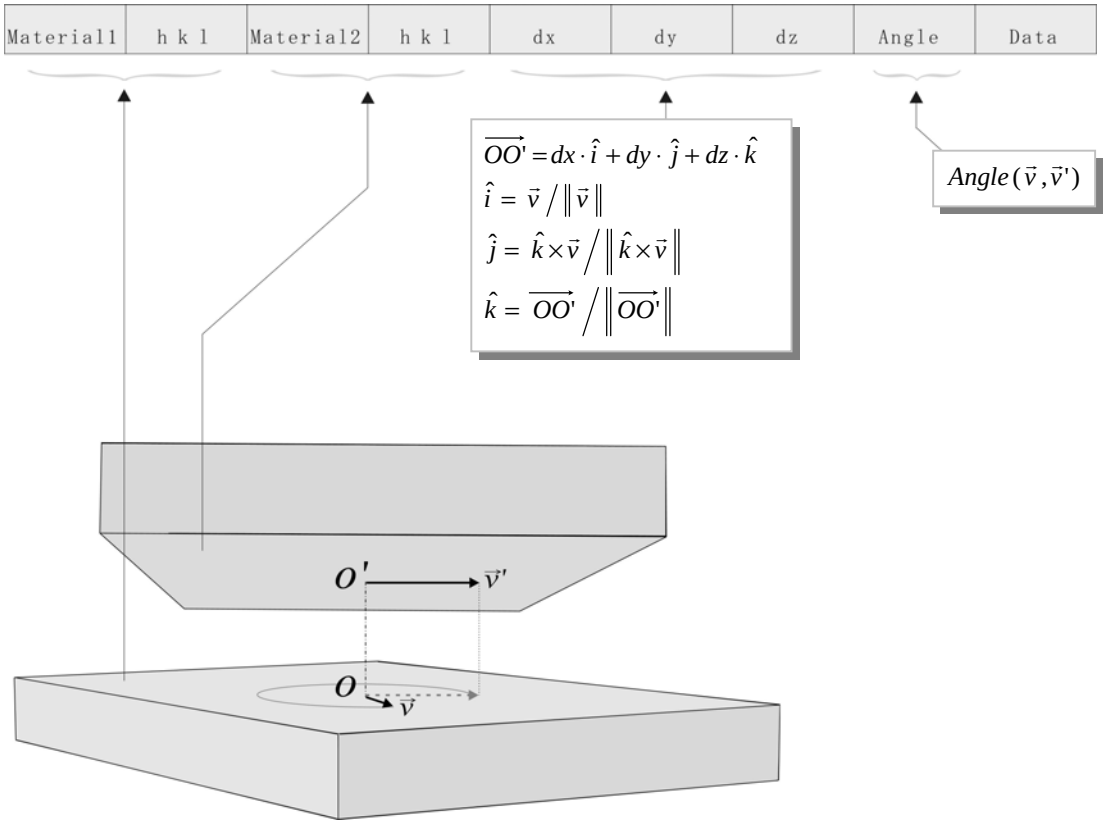

Figure 8. A typical database entry, the lower surface is set as the reference surface.

The *data* field might consist not only of a measurement(s) (or simulation outcome) but also of metadata. The metadata might contain details about how a measurement was obtained that are important to interpret the data. Since different users might need to store different data and/or metadata (including external files), some kind of flexibility is required in the repository. This requirement can be met by using an XML-Repository.

4.2 XML-Repository Example

Any document in XML format as defined in W3C (2003), can be checked against an XMLSchema. An XMLSchema is a set of *rules* that tell how to organize information contained in an XML document. If an XML document conforms to the *rules* described in a given XMLSchema it can be said that the XML document is valid (W3C, 2004) Schemas are used to check that XML documents abide to a standard.

An example of a copper interface in XML is shown in Table 2. The document displayed in Table 2 is valid (compatible) as per a XMLSchema called *datum.xsd* (TokyoTech, 2005). See Appendix 1. The *datum* element contains one *interface* element. Each *interface* element is described by 2 surface elements and at least one *data-set* element. The *data-set* element contains data (usually the outcome of a simulation) about a given geometry of the given interface. Each element might contain optional data and/or metadata elements defined by the user.

The proposed XMLSchema extensibility meets the flexibility requirements mentioned in 4.1, while its compulsory elements ensure a minimum of compatibility between repositories.

```
<?xml version="1.0" encoding="ISO-8859-1" ?>

<datum  xmlns  = "http://www.ide.titech.ac.jp/~jose/codata"
    xmlns:xsi = "http://www.w3.org/2001/XMLSchema-instance"
    xsi:schemaLocation="http://www.ide.titech.ac.jp/~jose/codata
    datum.xsd">

   <interface>
      <surface1>
         <material>Cu</material>
         <plane>1 0 0</plane>
      </surface1>
      <surface2>
         <material>Cu</material>
         <plane>1 1 1</plane>
      </surface2>
      <data-set>
         <dx>0</dx>
         <dy>0</dy>
         <dz>0</dz>
         <angle>10.5860</angle>
         <data>0.811</data>
         <measurementMethod>MEAM92</measurementMethod>
      </data-set>
   </interface>
</datum>
```

Table 2. Sample information of a copper interface in XML format

5 ACKNOWLEDGMENTS

This work has been supported by the *Inamori* foundation and in part by the Ministry of Education, Culture, Sports, Science and Technology of Japan under Grant-In-Aid for scientific research No.12875135.

6 REFERENCES

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6 APPENDICES

6.1 XMLSchema

```
<?xml version="1.0" encoding="ISO-8859-1"?>

<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema"
         targetNamespace="http://www.ide.titech.ac.jp/~jose/codata"
         xmlns="http://www.ide.titech.ac.jp/~jose/codata"
         elementFormDefault="qualified">

  <xs:element name="datum">
    <xs:complexType>
      <xs:sequence>
          <xs:element ref="interface"                          maxOccurs="unbounded" />
          <xs:element name="notes"           type="metadata"   minOccurs="0" />
          <xs:any minOccurs="0"/>
      </xs:sequence>
    </xs:complexType>
  </xs:element>

  <xs:element name="interface" >
     <xs:complexType>
       <xs:sequence>
         <xs:element name="surface1"         type="surface" />
         <xs:element name="surface2"         type="surface" />
         <xs:element ref="data-set"                           maxOccurs="unbounded" />
         <xs:element name="notes"            type="metadata"  minOccurs="0" />
         <xs:any minOccurs="0"/>
 </xs:sequence>
     </xs:complexType>
    </xs:element>

    <xs:complexType name="surface">
      <xs:sequence>
        <xs:element name="material"          type="xs:string" />   <!-- Fe, Cu,...         -->
        <xs:element name="plane"             type="xs:string" />   <!-- 1 1 0, 1 1 1,...   -->
        <xs:element name="cubicSystem"       type="xs:string"   minOccurs="0" />
                                                      <!-- bcc, fcc or cubic-diamond -->
        <xs:any minOccurs="0"/>
      </xs:sequence>
    </xs:complexType>

    <xs:complexType name="metadata">
      <xs:sequence>
          <xs:element name="source-author"   type="xs:string"    minOccurs="0" />
          <xs:element name="date"            type="xs:date"      minOccurs="0" />
          <xs:element name="note"            type="xs:string"    minOccurs="0" />
      </xs:sequence>
    </xs:complexType>

    <xs:element name="data-set">
      <xs:complexType>
        <xs:sequence>
          <xs:element name="dx"      type="xs:decimal" />  <!— see note 1 -->
          <xs:element name="dy"      type="xs:decimal" />
          <xs:element name="dz"      type="xs:decimal" /> <!-- by default Armstrongs -->
          <xs:element name="angle"   type="xs:decimal" /> <!-- by default deg  -->
          <xs:element name="data"    type="xs:decimal" /> <!-- by default Jm-2 -->
<xs:element name="xyzUnits"        type="xs:string"    minOccurs="0" />
          <xs:element name="angleUnits"      type="xs:string"    minOccurs="0" />
          <xs:element name="dataUnits"       type="xs:string"    minOccurs="0" />
          <xs:element name="measurementMethod"        type="xs:string"    minOccurs="0" />
          <xs:element name="notes"                    type="metadata"     minOccurs="0" />
        </xs:sequence>
      </xs:complexType>
    </xs:element>
```

```
<!--       note 1

       Reference point of Surface 2 ( O') =
       Reference point of Surface 1 ( O ) + dx*i + dy*j + dz*k ;

       i,j,k being unit vectors, where
       k is same direction as plane vector of surface1,
       i is orientating vector as per described Extended Unit Cell Method,
       j is same direction as the outer product of k with i

       angle is the amount of rotation on surface 1 that transforms the direction of v into v',
(a counter clock-wise rotation corresponds to a positive angle).
-->
</xs:schema>
```