Available online at www.sciencedirect.com

ScienceDirect

Procedia CIRP 54 (2016) 197 – 203

www.elsevier.com/locate/procedia

6th CLF - 6th CIRP Conference on Learning Factories

Atomistic modelling of interfaces in cold welded joints

Per Harald Ninive[a] *

[a]NTNU i Gjøvik, PO Box 191, Gjøvik NO-2802, Norway

* Corresponding author. Tel.: +47 61 13 52 59; *E-mail address:* per.ninive@ntnu.no

Abstract

Atomistic modelling is playing an increasingly important role as a tool to predict fundamental physical properties as well as mechanical properties of materials. With the steady improvement of powerful computational tools, increasingly realistic models can be employed in simulations of relatively complex systems. This has successfully been demonstrated for e.g. hardening precipitates in aluminium alloys. This approach should thus also be well suited for studying interfaces of metal-metal joints. In this paper, both possibilities and potential challenges of an atomistic modelling approach of such systems are discussed, with a particular focus on interface modelling of the industrially important Al-steel joints.

Peer-review under responsibility of the scientific committee of the 6th CIRP Conference on Learning Factories

Keywords: atomistic modelling; interfaces; aluminium; joints; density functional theory

1. Introduction

Multi-material components and technologies of joining components of different types of metals is a research area of great interest in modern automotive industry. An important example is the joining of aluminium components to steel in car bodies. In order to improve fuel efficiency, it is desirable to increase the use of lightweight components in cars. There are several different well-known techniques for joining metals, where traditional fusion welding is the most known and used. Although this method is suitable for steels, in aluminium a significant weakening of the material strength (e.g., softening, cracking, corrosion) due to microstructural changes around the fusion zone occurs after fusion welding or friction stir welding. Thus, cold welding techniques, in which the microstructure near the joint will be less affected are being considered, like the HYB (Hybrid metal extrusion & bonding) method [1, 2] or cold pressure welding (CPW) [3]. Improved knowledge of physical and mechanical properties of cold welded joints is thus desired. In addition to macroscopic properties that can be tested in laboratories, an increased knowledge of nanoscale properties, like e.g., elastic and shear strains and atomic bonding is crucial in order to obtain a complementary understanding of the properties of the joints. Such properties are in many cases not experimentally accessible, but can be predicted via theoretical models and simulations. With the steadily improving capacity of available supercomputers and numerical algorithms, increasingly large and complex atomistic models can be employed in simulations. So-called first principles (or ab initio) methods use a quantum mechanical treatment of electrons, thus providing an accurate approach based upon the laws of physics. This makes the methods very well suited for studies of e.g. chemical effects and elastic response at atomic level. However, the calculations are computationally demanding, as the computing time scales roughly as N^3, where N is the number of atoms in the model. At the present, models containing up to about 1000 atoms are feasible for first principles calculations. The most used and popular first principles based computational method is density functional theory (DFT) [4, 5]. Atomistic models containing the order of a few hundred atoms or more have scales comparable to continuum mechanics based models, and can thus be used in combination with these. This opens up the possibility of

Peer-review under responsibility of the scientific committee of the 6th CIRP Conference on Learning Factories
doi:10.1016/j.procir.2016.05.075

multiscale modelling, in which nanoscale properties found from the atomistic approach can be linked with classical models and provide macroscopic properties and parameters that are of relevance and interest for industrial applications. The gap between nanoscale models and macroscopic models is thus bridged.

List of abbreviations

CPW	cold pressure welding
HYB	hybrid metal extrusion & bonding
DFT	density functional theory
VASP	Vienna Ab Initio Simulation Package
FE	finite element
TEM	transmission electron microscopy
MD	molecular dynamics

2. Interface modelling

Interfaces play a very important role in governing mechanical properties of metals, such as e.g. strength and work hardening. Thus, modelling of various types of interfaces is a very active research area. In particular, grain boundaries are of interest, since they are sites of segregation of solute impurities and dislocations [6]. In addition, smaller interfaces, like those between hardening phases and a host metal matrix, which strongly affect the hardening mechanism in heat-treated alloys, have also been widely investigated (see e.g. [7, 8]). In the latter case, the interfaces are sufficiently small to be entirely included in first principles atomistic simulations, or in hybrid models, where atomistic first principles simulations are used in combination with classical models. On the other hand, the sizes of interfaces of welded joints are on an entirely different level of magnitude. Therefore, there have been less activity on atomistic modelling and simulation of such types of interfaces. Nevertheless, with the increased use of solid-state welding methods, increased knowledge of interface properties down to atomic scale is needed in order to develop and expand the use of such methods. This is particularly in order to make cold welding applicable for joining of dissimilar metals, like aluminium and steel.

2.1 Precipitate interfaces in Al-Mg-Si alloys

An example of the use of atomistic modelling and first principles calculations in combination with a continuum mechanical model was demonstrated in a recent study of hardening precipitates in Al-Mg-Si (6*xxx*-series) alloys [9]. These industrially important alloys gain a large increase in tensile strength due to the formation of needle shaped precipitates in the alloy during artificial aging [10, 11]. The length of the precipitates is typically about 50 nm and the width is typically 2-5 nm. The strain fields formed around these precipitates trap dislocations, which leads to mechanical strengthening of the alloy. The model consisted of a precipitate cross section embedded in an aluminium matrix (see Fig. 1b). The model thus included all relevant interfaces and corners (except the tips of the precipitate-needles). Excellent microscopy images of precipitate cross sections (see Fig. 1a), along with knowledge of the orientation relations between the crystal structures of the precipitate and aluminium, made it feasible to construct a realistic atomistic model.

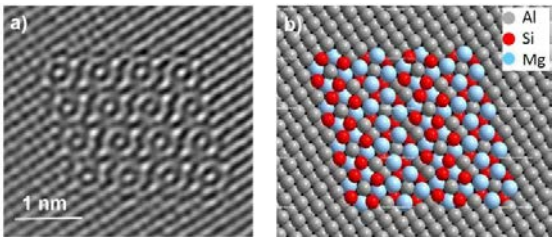

Fig.1. (a) TEM image of a precipitate cross section in an Al-Mg-Si alloy. Picture taken from ref. [12]. (b) Atomistic supercell containing a precipitate embedded in Al.

The atomistic model was then employed in a DFT calculation. In such calculations, the material structure is represented by so-called periodic supercells (as seen in Fig. 1b) repeated infinitely in all three spatial directions. It is therefore important that the supercell is large enough to contain all relevant strains and stresses due to the inserted precipitate, so that these are converged to approximately zero at the edge of the supercell. If this is not the case, the periodic images of the precipitates will "interact" with each other and lead to incorrect or inconsistent strain energies. In this model, the precipitates were represented as infinitely long needles. One such precipitate-matrix supercell typically contains between 500 and 1000 atoms, so a well-converged calculation thus requires a relatively large amount of computational resources. The DFT calculations were carried out using the VASP (Vienna *Ab Initio* Simulation Package) code [13, 14]. The most important outputs from these calculations are the relaxed atomic positions and the total free energy in the supercell, from which strain energies and interface energies can be obtained.

A similar classical precipitate model (with dimensions identical to those of the atomistic model) was then constructed and employed in a finite element (FE) calculation (see Fig. 2). The perhaps most obvious difference from the atomistic model is the precipitate-matrix interface, which was only represented as a straight and clean interface in the latter model. Among the main inputs in the FE model was the elastic coefficients of aluminium and of the precipitate, which were calculated separately using DFT. The easiest feature to compare in the two models is the simulated strain field in the Al matrix. This is also a quantity of high relevance when regarding the precipitates' influence on the mechanical strength in the alloy. Expectedly, the coherency strains simulated close to the interface and inside the precipitate did not correspond well with those simulated within the atomistic model. The main source of discrepancies was the way in which the precipitate-matrix interface was represented in the FE model. Electronic effects govern the elastic strains near the interface, so it must be treated quantum mechanically in order to provide a correct strain behaviour. The precipitate cross section was also small enough that the strains in its entire interior was affected by the interface. Nevertheless, a good agreement between the two models was found as long as the strains were considered at a sufficiently large distance