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Multiscale Simulations in Welds

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Abstract

Welding processes involve complex couplings between fluid dynamics, heat transfer and the metallurgical changes experienced by the base metal. Distortion, residual stresses, grain structure, cooling rates, high temperatures and consequently the reduced strength of a structure in and around a weld joint are produced by the localized thermal cycling caused by the intense heat input of fusion welding. With the virtual prediction of weld profiles (shape and size), solidification structures, distribution of impurities, formation of dislocations, distortions and residual stresses of a welded part, processes can be optimized in the early stages of prototyping.
The technological properties of fusion welds are formed due to the simultaneous effects of different physical phenomena which occur on different length scales. Correspondingly the simulation of technological properties of fusion welds requires the multiscale approach.

Keywords. Residual Stresses, Voronoi Cell Finite Element Modeling (VCFEM), Welding, Solidification; Dislocations.

Resumen

Los procesos de soldadura involucran acoplamientos complejos entre dinámica de fluídos, transferencia de calor y los cambios metalúrgicos que experimenta el metal base. Distorsión, tensiones residuales, estructura granular, tasas de enfriamiento, altas temperaturas y consecuentemente la resistencia reducida de una estructura en y alrededor de una junta soldada, son producidos por el ciclo térmico localizado causado por la intensa entrada de calor en soldadura de fusión. Con la predicción virtual de perfiles de suelda (forma y tamaño), estructuras de solidificación, distribución de impurezas, formación de dislocaciones, distorsiones y tensiones residuales de una parte soldada, los procesos pueden ser optimizados en la etapa temprana del diseño (prototipo). Las propiedades tecnológicas de las sueldas de fusión son formadas debido a los efectos simultáneos de diferentes fenómenos físicos los cuales ocurren a diferentes escalas. Correspondientemente, la simulación de las propiedades tecnológicas requiere la aproximación multiescala.

Palabras Clave. Tensiones residuales, Modelación Voronoi-Elementos Finitos, Soldadura, Solidificación, Dislocaciones.

Fusion welding processes are widely used for general repair applications. Successful repair requires the transient heat and fluid flow phenomena of the weld pool be addressed adequately to prevent the formation of new grains, equiaxed or columnar, ahead of the epitaxial columnar dendrites. It is well known that the dynamic behaviour of weld pools, due to heat and fluid flow in the weld pool, has significant influence on the temperature distribution, shape and size of the weld pool, final solidification microstructures, and consequently the resultant mechanical properties of the welded joints [1]. It is of great significance to understand the process quantitatively, focused on modelling the transient dynamics of the weld pool, especially the transient heating period after the arc ignites and the transient cooling period after the arc extinguishes to create specific solidification conditions.

Welding processes involve complex couplings between fluid dynamics, heat transfer and the metallurgical changes experienced by the base metal. The most critical input data required for welding fluid flow-thermal analysis are the parameters that describe the heat input to the weldment from the heat source [2, 3]. Distortion, resid-

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ual stresses, grain structure, cooling rates, high temperatures and consequently the reduced strength of a structure in and around a weld joint are produced by the localized thermal cycling caused by the intense heat input of fusion welding [2, 3]. With the virtual prediction of weld profiles (shape and size), solidification structures, distribution of impurities, formation of dislocations, distortions and residual stresses of a welded part, processes can be optimized in the early stages of prototyping. Predictions can be compared with experimental work to be feedback into the interacting model/weld fabrication system in order to optimize the welding process.

In ref. [3], it has been shown that where local models are sufficient to predict stresses, only global three-dimensional (3D) models can correctly predict distortions. In the 3D situation however, analysis of welding conditions has shown the presence of high temperature gradients leading to stresses and plastic strains in small areas, coupled with a varying microstructure. These factors necessitate the refinement of mesh size near the welding line, increasing drastically the models' size and consequently lead to unreasonable computation times. From a finite element point of view is not difficult to establish stable welding process using small geometric domains, so, small 3D global models that require small FE meshes can be used to correctly predict distortions. Physically based modeling of the entire three-dimensional (3-D) melt-pool geometry is a computationally formidable task. However, modeling the influence of the entire thermal cycle of the welding process with a physically based model for the material can provide new understanding of the microstructure and distortion evolution due to the welding process [4].

Differences in calculated and measured residual stresses are attributed to lack of an accurate stress-strain constitutive relation, experimental errors, and the use of Finite Element (FE) bulk coarse grids. The more textured the material, or the higher the intergranular stress (micro stress), or when there are chemistry changes, the less likely for measured and simulations to agree. An explanation could be that traditional welding simulations do not consider the polycrystalline nature of the specimen in the FE mesh step. Thus the uncertainties in the numerical calculations procedures include the inaccuracies in the calculation of thermal cycles as well as the approximations in the assumed stress-strain relation, particularly when important solid-state transformations take place [4, 5]. The critical first step in creating a science base not only for the repair applications but also for the design and analysis of welds, is to accurately compute the transient temperature field that lead to the formation of non equilibrium phases in and around the welded joint. Numerous welding problems, particularly those concerning with aircraft repair and fabrication, pressure vessels, piping and safety in the nuclear industry, are related to microstructure development and residual stresses [2]. The residual stresses that develop both in the fusion zone and heat-affected zone are detrimental to the integrity and service life of the welded part. Debroy and David [5] have shown that residual stresses can cause problems such as hydrogen-induced cracking and stress corrosion cracking, as well as distortion, initiate fracture and degrade the corrosion resistance of welded structures. Consequently, post weld heat treatment is often used to reduce residual stresses. Fracture mechanics based structural integrity assessments of pressure vessels and piping are widely used to support the economic and safe management of operating engineering plant. GTAW engineering techniques provide good quality, metallurgically bonded with a minimal heat input into the work piece. Although residual stresses have been studied for many decades, accurate calculation and measurement of these stresses still remains a major issue.

Computational models however can provide a detailed description of the residual stress distribution and microstructure development in weldments [4-6], though a prerequisite for the calculations is the detailed and accurate time-temperature history obtained from numerical simulations. Commercial software and in-house codes are used to simulate welding and joining processes. The predicted thermal, fluid and structural responses from these simulations are used for optimizing processes and carrying out structural integrity calculations. The technological properties of fusion welds are formed due to the simultaneous effects of different physical phenomena which occur on different length scales:

(i) Macroscopic (the order of magnitude of 0.1-1 mm): temperature distribution, temperature gradient, cooling rate, distortion, etc.;

(ii) Mesoscopic (the order of magnitude of 10-100 um): grain size, texture, plastic strains, strain gradients, residual stresses, etc;

(iii) Microscopic (the order of magnitude of 1-10 um): primary and secondary dendrite arm spacing, micro residual stresses, morphology, microsegregation, etc.

Correspondingly the simulation of technological properties of fusion welds requires the multiscale approach. The multi-scale analysis framework covers micromechanical stress and failure analysis, as well as thermal analysis, of extended microstructural regions. Problems solved by the Voronoi Cell Finite Element Method (VCFEM) range from heat transfer and stress-strain analysis of elastic, elastic-plastic, and viscoplastic material microstructures to microstructural damage models including interfacial debonding and ductile failure. Crack initiation typically starts at surface flaws or microstructural discontinuities, such as interfaces with second phase particles or grain boundaries. The geometry of the discontinuities and the orientation of the grains relative to the discontinuities play a critical role in crack initiation. Consequently, a model that captures these key relevant phenomena in order to predict crack initiation is mandatory.

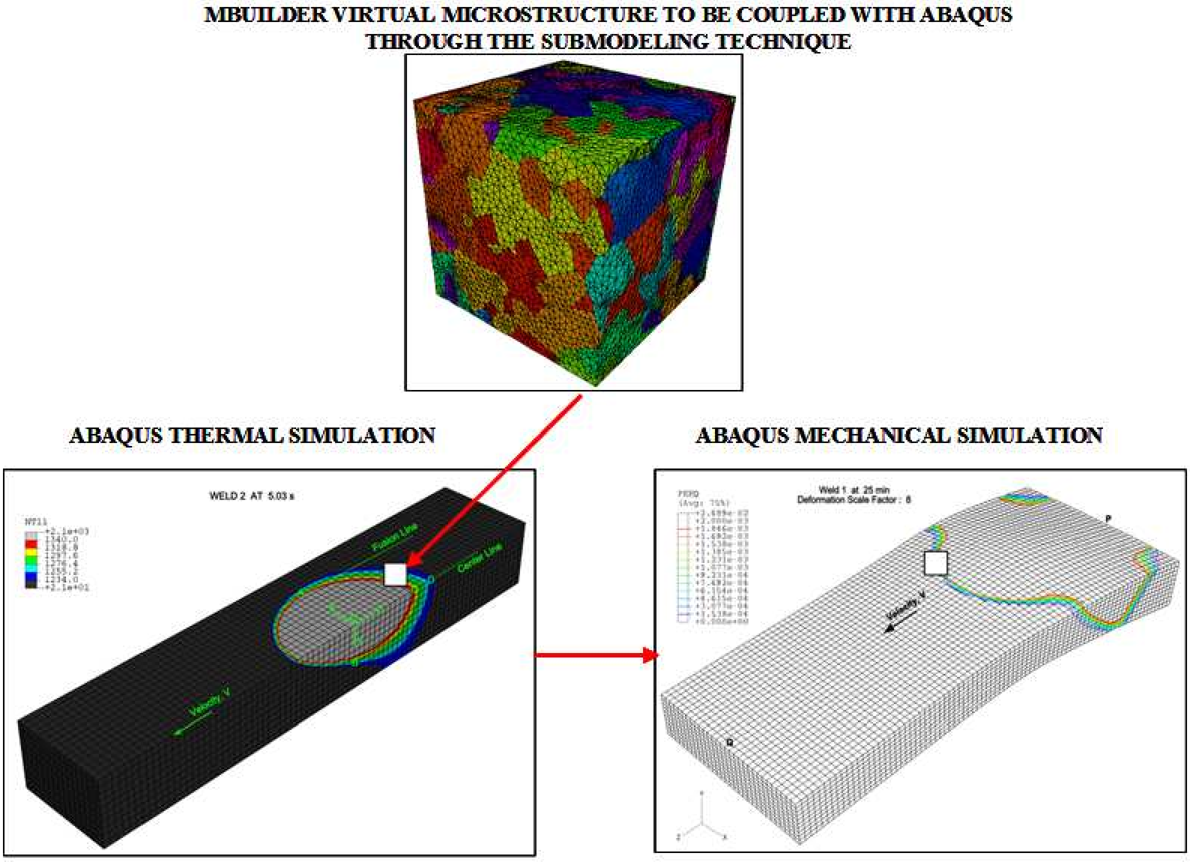

Figure 1: The Voronoi cell finite element physics-based model (a thermal-metallurgical-mechanical multiscale approach)

Heat flow during welding is of great interest to welding engineers and metallurgists. It not only controls the size of the fusion and heat-affected zones, but also strongly affects the microstructure and properties of the resultant weld. The temperature and velocity distributions of the molten metal as well as the cooling rate after welding operation affect the weld geometry, the microstructure, and the mechanical properties of weld zone. Near-perfect control of the temperature and heat flow distribution during welding crystallization (inside the weld pool) is essential not only to minimize distortion but also to control the distribution of impurities and the formation of voids and dislocations in the crystal lattice during cooling of the solid material. The crystallization process (welding microstructure evolution), the residual stresses (types I, II and III), the plastic strains and the dislocation density evolution are research fields of growing importance in the most prestigious research institutes around the world. The evolution of creep damage in the form of voids and cracks in a weld are related with dislocation emission and evolution. For instance, Lubarda et.al., [7] shown that the critical stress for the dislocation emission decreases with increasing void size, so that less stress is required to emit dislocations from larger than smaller voids.

As multi-phase metal/alloy systems are increasingly being used in industry, the science and technology for these heterogeneous materials has advanced rapidly. By extending analytical and numerical models, engineers involved with predicting the performance and failure of materials in structure-materials interactions, can analyze failure characteristics of the materials before they are integrated into the design process. In a previous work by Bonifaz and Richards [8], a thermal model to accurately generate weld profiles, analyze transient heat flow, and thermal cycles for three different welding speeds at constant heat input is clearly described. The thermal model developed was used to compute the transient temperature field, to predict solidification structures and to calculate the thermal gradient G and the growth rate R used to evaluate quantitatively the columnar to equiaxed transition in the GTAW process. Confidence was established in the model by comparison with theoretical, numerical and conventional phenomenological material models such as Kou [9], Norman et al, [10], Goldak et al, [11] and Goldak et al, [12]. For instance, thermal cycles at the weld centerline and fusion line reported in Kou [9], agree very well with the thermal cycles calculated in the mentioned work. Similarly, Paul and Debroy [13] correlated the calculated cooling rate in the weld pool with the secondary arm spacing. The cooling time through the solidification temperature range is shorter at the weld centerline and longer at the fusion line. As such, the cooling rate through the solidification temperature range increases and the dendrite arm spacing decreases from the fusion line to the centerline. In both the Kou [9] and Paul and Debroy [13] references, weld micrographs show the solidification microstructure gets finer from the fusion line to the centerline.

Epitaxial welding can be achieved on single-crystal (SX) components if adequate control of welding process is maintained, Norman et al. [10], Liu and Dupont [14], Park et al. [15], Richards et al., [16], Vitek, [17], Mokadem et al, [18] and Gaümann et al, [19]. It requires solidification theory for a close control of macroscopic heat input (epitaxy) and microstructure development to control the columnar to equiaxed transition (CET). Solidification must occur epitaxially from the underlying substrate without the nucleation of strays and/or equiaxed grains in the liquid. Melt-pool geometrical parameters which depend mainly on heat input have a profound influence on the dendrite growth velocity and growth pattern in the melt pool as demonstrated in Liu and Dupont [14], and Park et al, [15].

In Bonifaz and Richards [20], the mechanical model predicts highest residual stresses in regions of highest elastic strains, in agreement with conventional phenomenological material models where the macroscopic residual stress is always directly related to the macroscopic elastic strain. The highest residual stresses are located at the fusion line (where coarser dendrite secondary arm spacing exist); and the highest plastic strains are located at centerline (where finer dendrite secondary arm spacing exist). The mathematical modeling had been investigated with a view to generate numerical data to define an optimum Stress–Strain Evolution in Cast IN-738 Superalloy Single Fusion Welds parameter space to prevent the formation of cracks in the repair of gas turbine components. From the above observations, it appears that the strong plastic strain gradients at the centerline are directly related to finer dendrite arm spacing. However, no experimental attempt was made to demonstrate the strong size-dependence of plastic deformation in the micron range. It is important to point out that dendrite secondary arm spacing belongs to the micron-scale, while local plastic strains and residual stresses (type I) are considered to belong to the meso-scale, so a connection between the two scales is yet unclear. It is suggested that to clarify the link between scales, the effect of initial base metal microstructure (meso-scale) and dendrite secondary arm spacing (micron-scale) on geometrically necessary dislocations evolution need to be included in the analysis. In Bonifaz and Gil Sevillano [21], it was demonstrated that more dislocations are stored in specimens with finer grains and that the total dislocation density is not a single function of strain.

Experiments have shown that materials display strong size effects when the characteristic length scale associated with non uniform plastic deformation is on the order of microns. The classical plasticity theories cannot predict this size dependence of material behavior at the micron scale because their constitutive models possess no internal length scale. On the other hand, it is still not possible to perform quantum and atomistic simulations on realistic time and length scales required for the micron level structures [22]. A continuum theory for micron level applications is thus necessary to bridge the gap between conventional continuum theories and atomistic simulations [22]. A mechanism based theory of strain gradient plasticity based on a multiscale framework linking the microscale notion of statistically stored and geometrically necessary dislocations to the mesoscale notion of plastic strain and strain gradient is then necessary.

With all of the above in mind, the development of a physics-based model for simulating initiation and propagation of cracks in metal welded specimens, beginning at the microstructural length scale is necessary. The temperature predictions obtained from thermal-metallurgical models provide the "thermal loads" to the mechanical models. To predict dislocations however, the strain hardening model documented in ref. [23] could be inserted into the finite element mechanical analysis. Of this manner, the coupled thermal-metallurgical-mechanical model will handles time-dependent problems in three dimensions. This Voronoi Cell Finite Element Physics-Based Model (Fig. 1) will compute accurate stress, strain and dislocations fields in polycrystalline specimens under the welding processing conditions employed.

References

[1] Wu Ch. S.; Yan F. 2004. "Numerical Simulation of transient development and diminution of weld pool in Gas Tungsten Arc Welding." *Modelling Simul. Mater. Sci. Eng.* 12: 13–20.

[2] Bonifaz, E. A., 2000. "Finite Element Analysis of heat flow in single pass arc welds." *Welding Journal*. 79: 121–125.

[3] Bonifaz, E. A., 2007. "Thermo-Mechanical Modeling of Single Fusion Welds" *Canadian Welding Association Journal*. 1: 13–20.

[4] Thiessen R. G.; Richardson, I. M. 2006. *Metall. Mater. Trans. B.* 37B: 655–663.

[5] Debroy, T.; David, S. A. 1995. "Physical processes in fusion welding." *Reviews of Modern Physics*. 67: 85–112.

[6] Brown, S. B.; Song, H. 1992. "Implications of Three-Dimensional Numerical Simulations of Welding of Large Structures" *Welding Journal*. 71: 55–62.

[7] Lubarda, V.A.; Schneider, M.S.; Kalantar, D.H.; Remington, B.A.; Meyers, M.A. 2004. "Void growth by dislocation emission" *Acta Materialia*. 52: 1397–1408.

[8] Bonifaz, E. A.; Richards, N. L. 2009. "Modeling Cast In-738 Superalloy Gas-Tungsten-Arc-Welds" *Acta Materialia*. 57: 1785–1794.

[9] Kou S. 2003. "Welding metallurgy." 2nd ed. Wiley:, New York, NY.

[10] Norman, A. F.; Ducharme, R.; Mackwood, A.; Kapadia, P.; Prangnell P. B. 1998. "Aplication of thermal modelling to laser beam weldingof aluminum alloys." *Sci Technol Welding Joining*. 3: 260–266.

[11] Goldak, J. A.; Chakravarti, A. P.; Bibby, M.; 1984. "A new finite element model for welding heat sources." *Metallurgical Transactions*. 15B: 299–305.

[12] Goldak, J.; Bibby, M.; Moore, J.; House, R.; Patel, B. 1986. "Computer modeling of heat flows in welds." *Metallurgical Transactions*. 17B: 587–600.

[13] Paul, A.; Debroy, T. 1988. "Free surface flow and heat transfer in conduction mode laser welding." *Met. Trans. B*. 19: 851–858.

[14] Liu, W.; Dupont J.N. 2004. *Acta Mater.* 52: 4833–4838.

[15] Park, J.W.; Babu, S.S.; Vitek, J.M.; Kenik, E.A.; David, S.A. 2003. *J. App. Phys.* 94: 4203–4212.

[16] Richards, N.L.; Chaturvedi, M.C.; Liu, Y.G.; Mount K. 1996. *Int. J Mater. Prod. Technol*. 11: 284–290.

[17] Vitek, J.M. 2005. *Acta Mater*. 53: 53–60.

[18] Mokadem, S.; Bezenc, C.; Hauert, A.; Jacot, A.; Kurz W. 2007. *Metall Mater. Trans*. 38A: 1500–1510.

[19] Gaümann, M.; Bezenc, C.; Canalis, P.; Kurz, W.; 2001. *Acta Mater*. 49: 1050–1064.

[20] Bonifaz, E.A.; Richards, N.L. 2010. "Stress-Strain Evolution in Cast IN-738 Superalloy Single Fusion Welds." *International Journal of Applied Mechanics*. 2: 807–826.

[21] Bonifaz, E.A.; Gil Sevillano, J. 2000. "Modelo elasto-plastico de estructuras bifasicas policristalinas." PhD thesis, Escuela Superior de Ingenieros, University of Navarra, Spain.

[22] Gao, H.; Huang, Y.; Nix, W.D.; Hutchinson, J.W. 1999. *Journal of the Mechanics and Physics of Solids*. 47: 1239–1263.

[23] Bonifaz, E. A.; Richards, N. L. 2008. "The plastic deformation of non-homogeneous polycrystals." *Int. J. Plasticity*. 24: 289–301.