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Numerical Solutions for the Simulation of Heat-Induced Stress in Thin Film Materials

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Abstract:

Additive manufacturing and laser based fabrication techniques have become popular due to several reasons and utilize many thin film materials. These materials are subjected to intense localized heating during deposition, or processing, and understanding and predicting the thermal stresses and deformations that result from these various processes is a critical effort towards ensuring quality of the product and its performance. This article investigates leading edge numerical simulation methods for prediction of heat induced stress in thin films for the applications of laser cladding, droplet based manufacturing and other related technologies. Since thermal gradients, material properties, and geometrical constraints are complexly linked in thin film systems, sophisticated computational methods are required to accurately capture the underlying physics. Researchers and engineers can make valuable use of state of the art numerical techniques to get insight into stress evolution, deformation mechanisms and potential failure modes without the need for extensive and expensive experimental trials.

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1. Introduction

In Sections 2 and 3 the basic principles for heat transfer and stress generation in thin films are described, together with different simulation techniques and their applications to different manufacturing scenarios. This review includes a comprehensive overview that spans from coupled thermo mechanical models to advanced particle based techniques in order to enable readers to have a grasp on the state of the art in numerics for heat induced stress modeling in thin film materials. Fundamentals of Heat Transfer and Stress Development in Thin Films [1]-[4].

1.1 Thermal Conduction Mechanisms

During high temperature processing, thermal conduction is the primary mode of heat transfer in thin film materials. The heat flux through the material is controlled via Fourier's law where the heat flux is related to the temperature gradient within the material. In the thin film regime, the conduction behavior may be changed considerably in comparison with bulk materials due to the reduced dimensionality and the effects of interfaces. Anisotropic thermal conductivity in thin films is a common phenomenon where the in-plane and cross plane components of thermal conductivity differ. The source of this anisotropy comes from different grain structure, defects, and interfacial thermal resistance. Furthermore, thermal conductivity effective values decrease with the diminishing film thickness approaching the mean free path of heat carriers. Because of these complexities, the numerical simulations capable of accurately modelling heat transfer in thin films must take these into account. Commonly, finite element methods (FEM) and finite difference techniques are used to discretize the spatial domain, accompanying the heat equation with the appropriate boundary conditions. For example, when effects due to non-Fourier behavior must be captured at ultra-thin film scales or at very short time scales, more advanced approaches, including the Boltzmann transport equation may be necessary [5]-[8].

1.2 Thermal Expansion and Residual Stress Formation

Thermal expansion mismatch between the film and substrate produces considerable stresses as thin films go through temperature changes during processing or in operation. These stresses are dependent on a number of things such as the CTE difference, the elastic properties of the material, and the range of temperature the materials see.

There are three main categories of stress in thin films:

- Intrinsic stresses: Arising from the film growth process and microstructural evolution
- Thermal stresses: Induced by CTE mismatch and temperature gradients
- Extrinsic stresses: Resulting from external loads or environmental factors

In order to capture the thin film's stress strain behavior under thermal loading, the numerical simulations must be appropriate with the constitutive models. The theoretical basis for most of these models is generally based on the elasticity theory, although plasticity, creep, or viscoelastic effects needs to be incorporated in a more sophisticated manner for certain material systems and temperature regime [9].

2. Influence of Microstructure and Interfaces

The thermal and mechanical properties of thin films are controlled by the microstructure, the grain size, the texture and the defect density. Sources, (and sinks) for defects, and mechanisms of stress relaxation depend on all interfaces between the film and the substrate and also on grain boundaries within the film itself.

The microstructural aspects must be taken into account in these models for predicting heat induced stress in thin films. Over the last few decades there has been a growing interest in integrating atomistic simulations with continuum mechanics to constitute multiscale modeling approaches in order to account for the interplay between microstructure within the framework of material behavior. These methods provide a more realistic model of phenomena such as grain boundary sliding, dislocation motion and diffusional creep [10]-[11].

2.1 Coupled Thermo-Mechanical Simulation Techniques

Finite Element Analysis for Thin Film Systems. Finite element analysis (FEA) has proven to be a versatile simulation tool suitable for simulating such coupled thermo-mechanical behavior of thin film materials. The geometry is discretized into small elements to solve complex partial differential equations governing heat transfer and growth of the stress. In the present discussion of thin films, steps usually involved in FEA models are:

- Geometry creation and meshing: The film-substrate system must be represented in terms of the appropriate element types and mesh refinement.
- Material property definition: Assigning temperature-dependent thermal and mechanical properties to each component
- Specification of boundary conditions: Heat input, cooling condition and mechanical constraint

Selection of appropriate numerical algorithms for coupled thermo mechanical problem. Extracting relevant data of temperature distributions, stress fields and deformation patterns, post processing and analysis. Dedicated thin film modules are available within commercial FEA software packages such as ABAQUS, ANSYS and COMSOL, or alternatively open-source solutions, such as for example FEniCS offer flexibility to formulate a custom model and solver [12]-[14].

2.2 Time-Dependent Analysis and Transient Effects

Several thin film processing techniques require rapid heating and cooling cycles, which means that transient analysis of the thermal and mechanical effects needs to be considered during their time dependence. The common methods for solving the coupled equations of heat transfer and structural mechanics are implicit and explicit time integration schemes. According to the backward Euler or the Newmark-β schemes, implicit methods are unconditionally stable, but a system of equations must be solved at each time step. Central difference method is an explicit method which is computationally cheap for small time steps but might lose stability for larger sizes. The implicit versus explicit choice depends on the time scale of interest and other factors such as material properties and the nature of the loading conditions. To enhance accuracy and computational efficiency with problems of rapid temperature changes or nonlinear material behaviour, adaptive time stepping algorithms can be incorporated [15]-[16].

Table 1: Simulation Parameters for Heat-Induced Stress Analysis

Parameter	Value	Unit	Description
Film thickness	1	µm	Thickness of the thin film
Substrate thickness	500	µm	Thickness of the substrate
Initial temperature	25	°C	Ambient starting temperature
Maximum temperature	250	°C	Peak temperature applied during simulation
Thermal conductivity (film)	130	W/m·K	Thermal conductivity of the film material
Thermal conductivity (substrate)	1.5	W/m·K	Thermal conductivity of the substrate
Coefficient of thermal expansion (film)	2.6×10−6	1/K	Linear thermal expansion coefficient of the film
Young's modulus (film)	180	GPa	Elastic modulus of the film
Poisson's ratio (film)	0.3	–	Assumed isotropic behavior
Time step	0.01	s	Time increment used in simulation

3. Nonlinear Material Models and Large Deformation Analysis

Large deformations and nonlinear material behavior may be significant if thin films experience extreme temperature gradients and potentially high stresses during processing. It is necessary to include appropriate constitutive models in these numerical simulations in order to capture these effects accurately. Potential material models include non linear material models for thin films. Geometric nonlinearities must be accounted for by the use of updated Lagrangian or total Lagrangian formulations for large deformation analysis. The main benefit is that these approaches ensure equilibrium equations are satisfied in the deformed configuration, especially valuable if significant shape changes or buckling are involved [17]-[19].

3.1 Advanced Particle-Based Methods for Thin Film Simulations

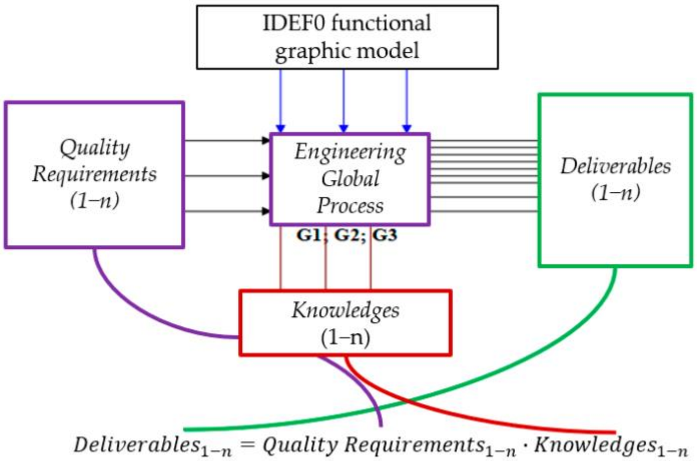

Fig. 1. Thermal Analysis Smoothed Particle Hydrodynamics (SPH)

Since the introduction of smoothed particle hydrodynamics (SPH), it has become a meshless method of interest for performing complex fluid dynamics and heat transfer problems. SPH is appealing for the thermal behavior modeling of thin film materials because of several of its advantages, for instance, in large deformations and free surfaces.

The fundamental principle in SPH is that of unveiling continuum as a set of discrete particles and therefore, each particle would carry mass, velocity and temperature. A thermal conductivity model is implemented by a smoothing kernel function defined on particle interactions [20]-[25].

Integration of SPH with Finite Element Methods

SPH is a great method for simulating fluid like bebaivors and heat transfer but may not be the most efficient technique for simulating solid mechanics in thin film substrates. In order to overcome this disadvantage, hybrid SPH-FEM schemes, which exploit the virtues of both methods, were introduced by researchers. In these coupled simulations the coupled physics are realized by using SPH particles to represent the deposited material (or fluid) phase and with finite elements for the substrate. Appropriate coupling algorithms are used to make the interaction between the two domains, keeping temperature and heat flux continuity at the interface.

Coupled SPH-FEM simulations present challenges in implementing in which new robust and stable coupling schemes need to be developed for the cases of high speed impacts and rapid solidifiction. Issues with these problems can be addressed and computational efficiency improved by using adaptive refinement techniques and multi-time steppping algorithms.

3.2 Molecular Dynamics for Nanoscale Thermal Transport

However, as thin film thicknesses get down to the nanoscale, there will be some continuum based methods will start to break down because the atomic scale effects become more important. Taken together, MD simulations provide a powerful tool to study thermal transport as well as stress development at nanoscales. But MD simulations are computationally expensive and apply only to small system sizes and short time scales. Multiscale modeling approaches that bridge gaps between atomic and continuum scales by linking MD with coarse grained or continuum methods have been devised [26]-[29].

4. Applications in Laser Cladding and Additive Manufacturing

Heat source modeling: Representing the laser beam as a moving heat source with appropriate intensity distribution. Powder feed dynamics: Simulating the interaction between the powder stream and the melt pool.

4.1 Melting, solidification, latent Heat

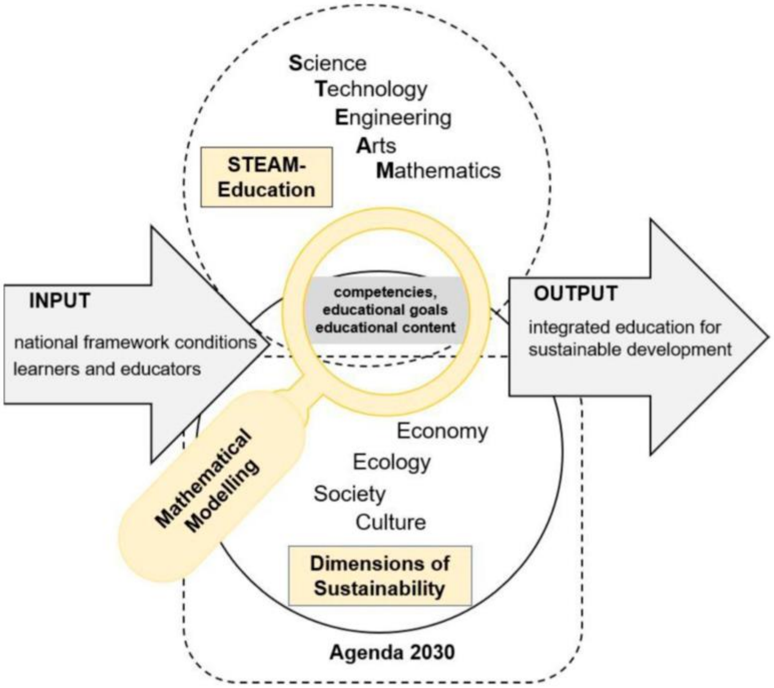

Fig. 2. Fluid flow in the melt pool: Modeling convection and surface tension-driven flows

Combined SPH-FEM approach has proved to be an advanced simulation technique to capture the intricate physics of laser cladding processes. Modeling for these cases allows for understanding of melt pool dynamics, thermal gradients, cooling rates and their relationship to microstructure evolution and residual stress formation.

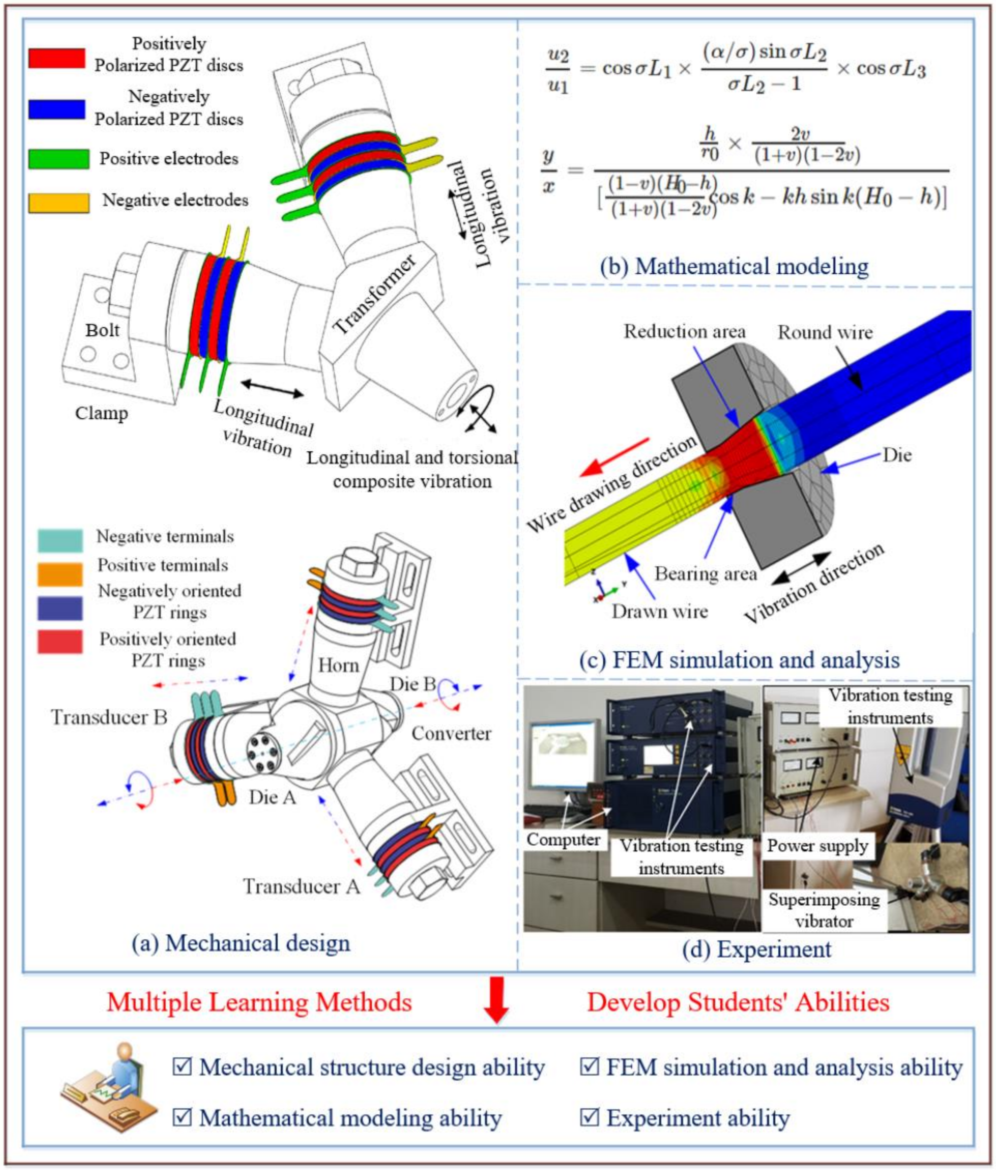

Fig. 3. Residual Stress Prediction and Deformation Analysis

Laser cladding induces residual stresses that may create cracking, delamination or substrate distortion. The predictions and mitigation of these issues rely on numerical simulations. Due to predictions of residual stress distributions and resulting deformations through coupled thermo-mechanical simulations, usually accomplished using FEA, mechanical performances are predicted. The models are typically elasto plastic and, where material undergoes phase transformation associated with processing, the kinetics of the phase transformation are also included.

4.2 Optimization of Process Parameters and Path Planning

Laser cladding process parameters optimization as well as path planning design can be valuable using numerical simulations. In a world of limited funds available for physical testing and exploration, researchers and engineers can conduct virtual experiments to explore a huge range of processing conditions before ever doing an expensive physical trial. Coupled with numerical simulations, advanced optimization techniques as genetic algorithms or machine learning approaches can be used to explore the parameter space and find the optimal processing conditions with a limited number of simulations. The goal of path planning optimization is to minimize the heat accumulation and reduce overall part deformation. New strategies for scanning have been developed through simulation approaches driven by.

4.3 Alternating between sectors of the cladding area

Material deposition of small island regions to distribute heat input. Dynamic scanning pattern: Changes the scanning pattern on the fly based on local thermal conditions. These optimized strategies have yielded promising WRR reduced residual stresses and overall part quality in laser cladding and similar AM processes [30]-[32].

5. Challenges and Future Directions

5.1 Multi-Physics Coupling and Scale Bridging

Currently, as the complexity of thin film manufacturing processes continues to grow, there is a need for multi physics simulation that can capture interplay of thermal, mechanical, and micro structural phenomena. Future research in this area may include:

- Development of efficient coupling schemes for thermal, fluid, and solid mechanics solvers
- Coupling of phasefield models for microstructure evolution in continuum scales
- Adaptive multi-scale frameworks seamlessly enabled by implementation of appropriate atomic, mesoscale, and macroscale representations.

These advances will support more complete, more accurate prediction in thin film materials of the magnitude and timing of heat induced stress/deformation over a broad range of length and time scales [33].

Table 2: Computed Thermal Stress in Thin Film Over Time

Time (s)	Temperature (°C)	Thermal Strain	Stress (MPa)	Stress Type
0	25	0	0	None
5	75	0.00013	23.4	Tensile
10	125	0.00026	46.8	Tensile
15	175	0.00039	70.2	Tensile
20	225	0.00052	93.6	Tensile
25	250	0.00058	104.4	Tensile

6. High-Performance Computing and GPU Acceleration

Efficient parallel algorithms and hardware acceleration techniques are needed for the solution of coupled thermo-mechanical simulations, especially from large scale or high resolution models. Future efforts may include:

- Optimization of existing numerical methods for massively parallel architectures
- Development of novel GPU-accelerated solvers for specific thin film simulation scenarios
- Hybrid CPU-GPU algorithm implementation to balance computational load with memory usage

They will allow, for instance, faster turnaround times for complex simulations, and thus useful real time process monitoring and control in industrial settings [34]-[35].

6.1 Machine Learning Integration and Surrogate Modeling

While the integration of machine learning techniques with numerical simulations holds great promise for improving the efficiency and predictive potential of heat induced stress models, there are still significant time and effort required to prepare the model, and to couple with LSS data. Potential applications include:

- Rapid approximation of complex simulation results using surrogate models
- Physics informed neural network implementation for solving partial differential equations
- Utilization of reinforcement learning algorithms for process parameter optimization

Data driven approaches enable researchers to speed up the discovery of new materials and thin film manufacturing processes.

7. Conclusion

While the numerical solutions for simulating heat induced stress in thin film materials have come a long way, enabling us to gain powerful tool in understanding and optimizing complex manufacturing processes. The field is still undergoing fast changes, involving among other techniques advanced finite element techniques, particle based methods and multi scale approaches. Looking to the future, high performance computing, machine learning and multi physics coupling integration should enable the limits of what is possible in thin film stress prediction. These developments not only advance our fundamental knowledge regarding material behaviour but also allow the advent of creative manufacturing technique and produce performance in almost every plausible application. We can unlock new possibilities in the field of thin film engineering and advance to more areas such as microelectronics and advanced materials, if we stand to embrace these emerging technologies and continue improving or simulation methodologies.

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