Mechanistic Analysis of Interfacial Bonding of Cold Sprayed Metallic Particles Using Smoothed Particle Hydrodynamics Method

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URL	http://hdl.handle.net/10097/61683

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授与学位	博士（工学）
学位授与年月日	平成23年9月14日
学位授与の根拠法規	学位規則第4条第1項
研究科，専攻の名称	東北大学大学院工学研究科(博士課程)機械システムデザイン工学専攻
学位論文題目	Mechanistic Analysis of Interfacial Bonding of Cold Sprayed Metallic Particles Using Smoothed Particle Hydrodynamics Method (Smoothed Particle Hydrodynamics 法を用いたコールドスプレー金属粒子の界面接合メカニズム解析)
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論文内容要旨

Cold spray (CS) is a materials deposition process in which relatively small particles of size range between 10 and 50 μm are accelerated in a supersonic inert gas flow and subsequently develop a coating on an appropriate substrate or a deposited layer of material by an impaction process. The distinguishing feature of the cold spray process is its ability to produce coating formation from particles in a solid state by accelerating the powder particles at a temperature that is always lower than the melting point of the material. The main coating characteristics minimize the effects of high temperature on coatings and substrate commonly associated with thermal spray methods, which include low porosity level, low oxidation, good adherence between the substrate and the coating, increased hardness, phase transformation, absence of microstructural changes, and lack of grain growth. It is generally accepted that adiabatic shear instabilities developing at the interface during impact is responsible for successful bonding, however there is little common agreement as to what interfacial reaction is the most dominant for bonding. In spite of the numerous studies conducted on the CS process, the actual mechanism by which the particles deform and bond is still unknown. The objective of this study is to investigate the dominant bonding mechanism of the CS technique through both numerical simulation and experimental measurement.

Chapter 1 is an introduction of the cold spray process. This chapter covers the literature review, previous researches and the goals of the thesis. The information provided in the literature review was used in the initial planning stages of the project.

In Chapter 2, the CS process was simulated by modeling the impact of spherical aluminum powder particles onto aluminum substrate over a wide range of velocity using the Smoothed particle hydrodynamics (SPH) method. The Dugdale-Barenblatt cohesive zone model was for the first time used to describe adhesive interaction between the contacting surfaces. Previous numerical models were only capable of predicting the critical velocity. However in this study, the proposed SPH model in Chapter 2 has enabled a good prediction of the particle velocity range for optimum deposition. The reliability of the model was verified through CS experiments of single particle impact tests in Chapter 3. The deformation pattern of Al powder particle during impact obtained using SPH and experiments are given in Fig. 1. The effect of velocity on the particle deformation behavior was analyzed and a rebound phenomenon was observed. The critical and maximum velocities were estimated with respect to these numerical and experimental analyses given in Fig. 2. The SPH model was also tested by simulating CS results already published.

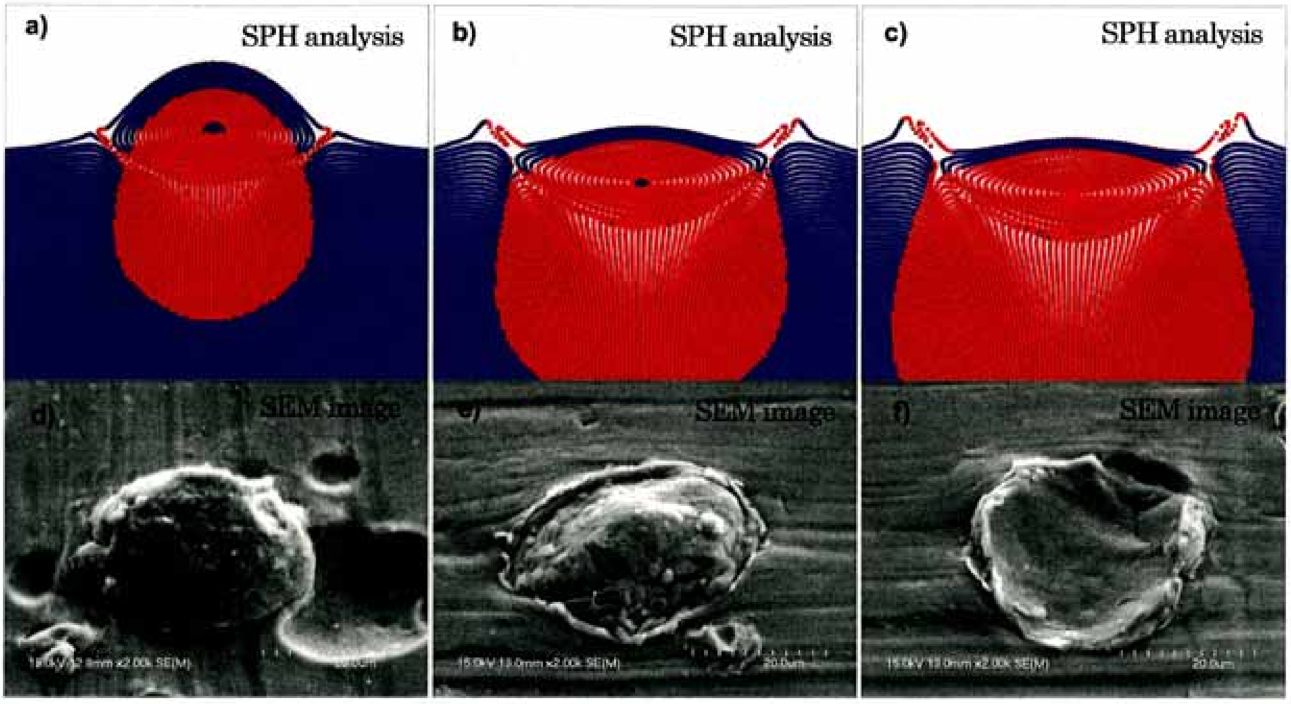

Fig. 1: The deformation pattern of Al powder particle during impact at a,d) 700 m/s b,e) 780 m/s and c,f) 840 m/s

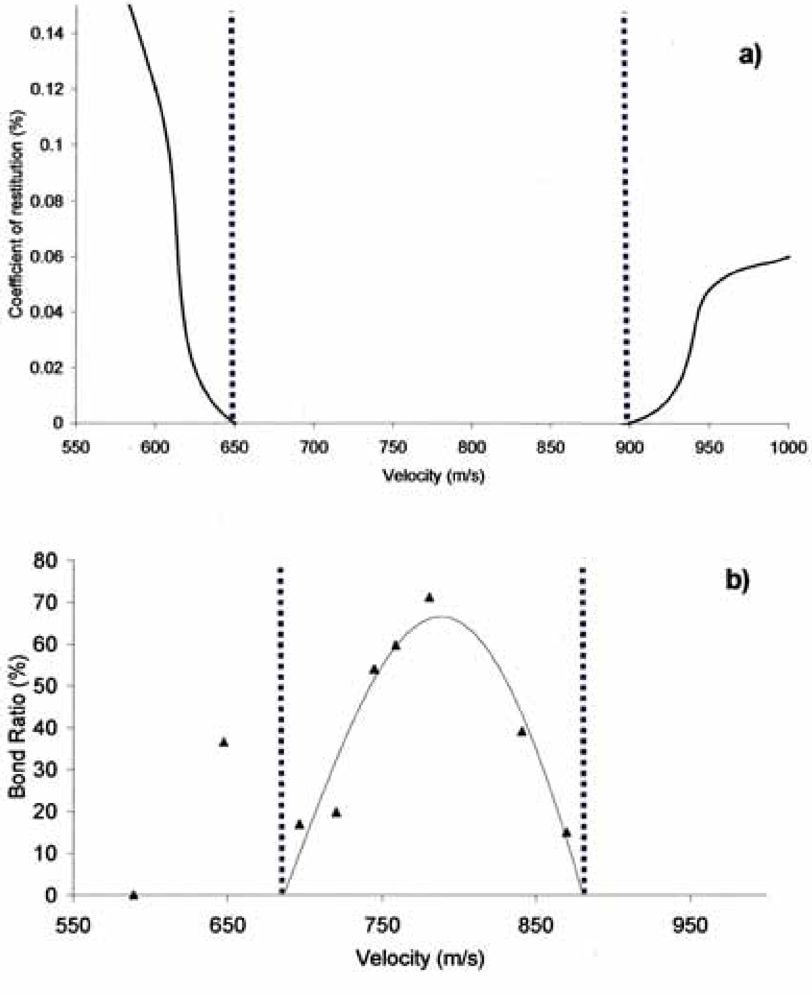

Fig. 2: The critical and maximum velocities obtained using a) SPH and b) experiments indicated by dashed lines.

In order to understand and explain the particle velocity range for optimum deposition, analysis with respect to the rebound and deposition energy was conducted in Chapter 4. In this chapter, the impact of cold sprayed particles is simulated using various metals. The materials are classified into four impact cases (soft/soft, hard/hard, soft/hard, and hard/soft), according to their physical and mechanical properties. The impact behaviors of each case are numerically analyzed using SPH. These analyses include the impact shape, the coefficient of restitution, and the rebound and deposit energy ratio, which can be combined together to identify the critical, maximum and optimum velocity. It was revealed that besides the critical velocity, the minimum velocity for deposition to occur, it is important to take into account the maximum velocity, the maximum velocity for deposition before the particles start rebounding, and the optimum velocity, the velocity at which the highest deposition efficiency is achieved. Estimating the maximum velocity and the optimum velocity was previously only possible by experiments. Thus the work here can substantially reduce the task of process optimization and thus contributes to the development of cold spray process. The influence of powder and substrate material and particle size on the critical, maximum, and optimum velocity is also discussed. The optimum velocity is not influenced by the number of impacting particles. This indicates that the analysis of a single splat is sufficient enough to determine the critical velocity, maximum velocity and the optimum velocity for a certain particle/substrate combination.

Thermal barrier coatings (TBCs) are widely used in gas turbines to increase their efficiency. A TBC consists of a metallic bond coat and a thermally insulating yttria-stabilized zirconia (YSZ) ceramic top coat. During service, a thermally grown oxide (TGO) that consists predominantly of alumina develops and continues to grow between the top coat and the bond coat. Past work has shown that the formation of TGO plays a crucial role in the failure of TBC. One of the commonly observed failure mechanisms is the oxide spallation at the TGO/YSZ interface, which is initiated by rapid and uneven TGO growth and formation of mixed oxide at the TGO/YSZ interface. Non-uniform growth of the TGO layer caused by the different thermal expansion coefficient between the TGO and the top coat, introduces a very high residual compressive stress field followed by cracking at the TGO/YSZ interface. To improve TBC performance and durability, a stable, continuous, slow-growing and adherent TGO scale during the entire period of oxidation is preferred. Several papers reported that desirable TGO properties could be achieved by modifying the bond coat properties. These properties are particularly dependent on the pore morphology, which in turn depends upon the coating process. Generally, bond coats are deposited by means of thermal spray techniques. These techniques, however, produce coatings with high initial oxide content, which results in high oxide growth rates when subjected to high temperature oxidation. Therefore in order to produce bond coats with high oxidation resistance and improve oxidation behavior, an alternative coating technique should be considered.

In Chapter 5, the analysis developed in Chapter 4 is applied to study the as-sprayed coating properties and microstructure and oxidation behavior of TBC with APS-YSZ top coat and CoNiCrAlY bond coat deposited using CS at the optimum velocity obtained using the SPH analysis. The coatings were subjected to isothermal oxidation and creep tests and evaluated using scanning electron microscopy (SEM), energy dispersive X-ray spectrometry (EDX) and transmission electron microscopy (TEM), and electron backscattered diffraction (EBSD). The microstructure of the as-sprayed bond coat is given Fig. 3. It was found that the bond coat was less porous. The pores found within the bond coat are typically small with an average diameter of 100 nm. This indicates that sufficient plastic deformation of impinging particles upon impact is achieved and conversely the bonded particles have sufficient kinetic energy to achieve adequate plastic deformation.

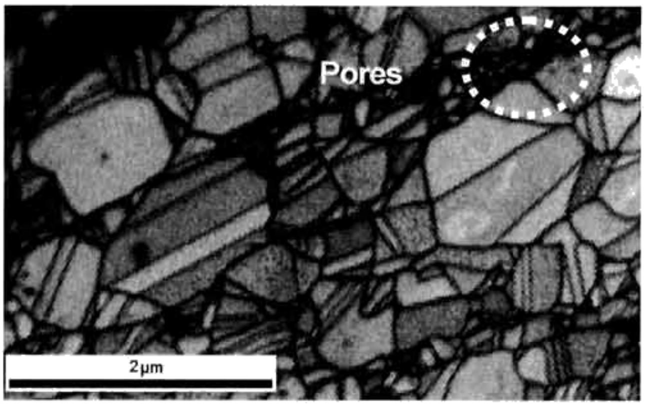

Fig. 3: EBSD image of as-sprayed CoNiCrAlY bond coat.
(Pores are indicated by the dotted circle.)

The microstructures of the oxidized TGO are given in Fig. 4. The oxidation study revealed remarkable results. The oxides observed in the TBC was an undulated TGO composed of predominantly alumina. These results demonstrate that while the deposition techniques that limit the initial oxide content may result in an improvement of the oxidation behavior of the coating. The quality can be maximized by optimizing the initial spray condition to obtain the optimum velocity. Thus, high quality bond coat that forms a stable and continuous alumina can be produced by the CS deposition technique, preferably at the optimum particle velocity.

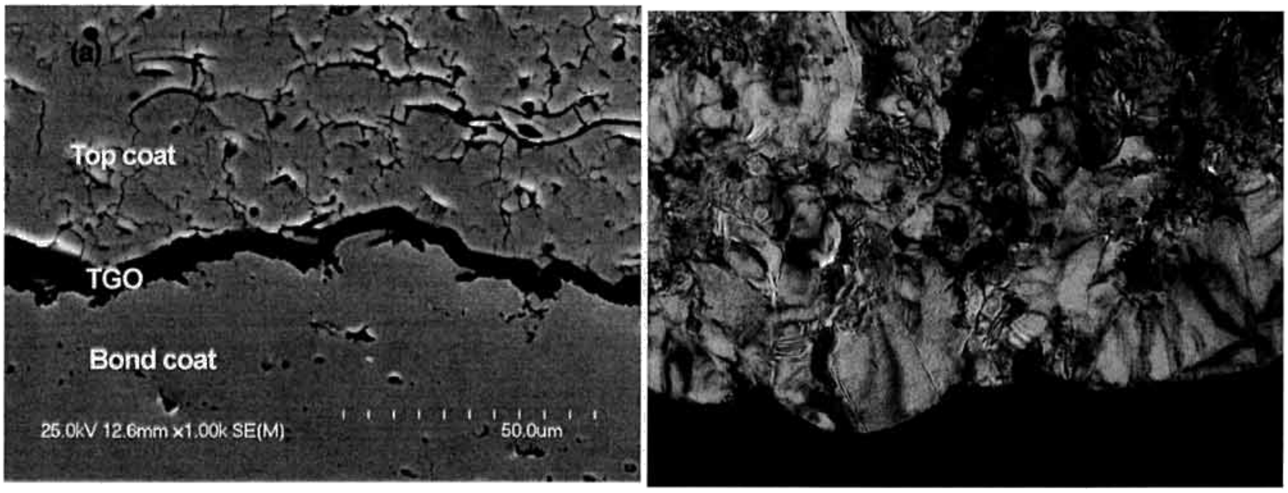

Fig. 4: (a) SEM image and (b) TEM image of TGO microstructure after oxidation at 900 °C for 800 h without creep

The conclusions of the thesis are provided in Chapter 6. Surface adhesion driven by intersurface forces is proposed as the bonding mechanism. Adhesion is an atomic length-scale phenomenon and its occurrence is controlled by the presence of clean surfaces and high contact pressures to make the two surfaces mutually conforming. Therefore the formation of a mutually conforming contact surface is an indication of attractive atomic interaction. This attractive atomic interaction was translated to a larger scale, and modeled in SPH as forces acting at the contact surface, upon impact. Results obtained using SPH was in good agreement with experiments and published results. Therefore it can be concluded that interfacial bonding may be driven by the intersurface forces that acts within the cohesive region.

論文審査結果の要旨

コールドスプレー(CS)法は，金属粒子をヘリウム等のガスで加速し溶融させることなく基材上へ衝突させて成膜する手法であり，施工中の酸化や相変態がほとんど発生しないといった特徴からコーティングの形成や補修等への応用が期待されている。成膜における粒子付着に関しては，粒子速度が大きく影響し，ある速度を境に付着が開始し，さらに速度が上昇すると粒子は反発し付着しなくなる。この粒子付着速度域を求めることは信頼性に優れたコーティングや補修部を得るために必要不可欠であるが，これは実験により求めるしか方法は無く，さらに粒子や基材材料によっても速度域は異なるため，膨大な労力と時間を費やすことになる。

本論文は，上記の問題を解決するために，CS 法における粒子／基材接触界面の接合に対し，粒子法の一つであるSmoothed Particle Hydrodynamics (SPH)法の応用に焦点をあてた研究の成果をまとめたものであり，全編6章からなる。

第1章は序論であり，本研究の背景，目的および本論文の構成を述べている。

第2章では，CS法における粒子の付着および反発を評価する上で最も重要なSPH 法の解析モデルを構築しており，とりわけDugdale-Barenblatt cohesive zoneモデルをSPH法へ応用することにより，粒子の付着・反発の評価が可能であることを世界に先駆けて明らかにしている。また，本手法により，CS法における粒子の付着に最も重要な粒子付着速度域の推定を可能にしている。この成果は，粒子の付着解析に対し新たな学術的解釈をもたらす工学上重要な知見であるばかりでなく，工業上も有効な知見を与える極めて重要な成果である。

第3章では，実験による粒子の付着挙動とSPH法による解析の比較を行っており，SPH法による解析結果が実験による粒子変形挙動を正確に捉えていることを検証し，SPH法の妥当性を述べている。また実験結果から，粒子の付着効率が最大となる最適粒子速度の存在を明らかにしており，極めて実用性の高い成果を得ている。

第4章では，SPH法と粒子の付着エネルギー・反発エネルギーの関係から，粒子付着速度域ならびに第3章で得られた最適粒子速度を定量的に評価することに成功している。CS法においては粒子速度のみでなく粒子の大きさや基材の種類も粒子付着に対し重要なパラメーターとなるが，本手法の応用により，粒子付着に及ぼす粒子径の影響および粒子材料／基材材料の組み合わせによる粒子付着速度域および最適粒子速度の評価も可能としており，実用上有用な新しい評価手法を提案している。この成果は，付着性の高い成膜に対し重要な指針を与えるものである。

第5章では，SPH法の応用例として，既存の研究成果に対してCS法における成膜結果とSPH法による解析結果を比較し，両者の良好な一致を得るばかりでなく，他の研究者らの成膜条件の有効性に対し学術的な解釈をもたらしており，有用な成果である。

第6章は結論である。

以上要するに本論文は，コールドスプレー法における金属粒子の付着に対し，SPH法を応用することで，粒子付着に最も重要な粒子付着速度域および付着効率の最も高くなる最適粒子速度の推定を可能にしたばかりでなく，粒子／基材界面の付着挙動に関する基礎的な学術的解釈を与えており，機械システムデザイン工学及び表面改質工学の発展に寄与するところが少なくない。

よって，本論文は博士(工学)の学位論文として合格と認める。