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Shape Memory Polymer Nanocomposites for Application of Multiple-Field Active Disassembly: Experiment and Simulation

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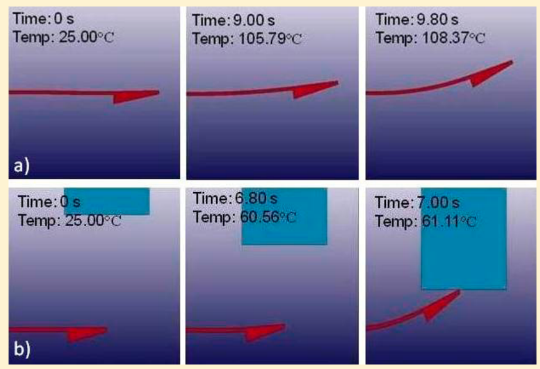

ABSTRACT: Active disassembly (AD) uses innovative materials that can perform a designed disassembly action by the application of an external field. AD provides improvements over current disassembly processes by limiting machine or manual labor and enabling batch processing for end-of-life products. With improved disassembly operations, more reuse of components and purer recycling streams may be seen. One problem with AD, however, has been with the single-field actuation because of the probability of accidental disassembly. This presentation will discuss the application of shape memory polymer (SMP) nanocomposites in a new AD process. This novel AD process requires multiple-field actuation of the SMP nanocomposite fastener. In the analysis of this AD process, thermal and magnetic field tests were performed on the SMP nanocomposite. From these tests, finite-element analysis was performed to model and simulate the multiple-field AD process. The results of the simulations provide performance variables for the AD process and show a better performance time for the SMP nanocomposite fastener than for a comparable SMP fastener.

■ INTRODUCTION

Product disassembly has not been a popular end-of-life (EoL) activity mainly because of the high cost of disassembly operations and low benefits gained from post-disassembly operations (e.g., resell of materials and/or components from recycling, remanufacture, reuse, etc.). With the current focus on the environment, disassembly is becoming a heavily promoted, if not mandatory, EoL activity because of the environmental benefits that can be gained by disassembly. For example, disassembly allows for the proper disposal of hazardous materials within product assemblies. Disassembly also promotes reuse of products and components and allows for purer recycling of product materials.[1] Because of such benefits, industrial and governmental initiatives motivate manufacturers to overcome the cost disadvantages and disassemble.[2] In doing so, research has focused on ways to make disassembly more economically viable to reduce the economic burden on manufacturers.

Active disassembly (AD) has become the avenue that would make EoL product disassembly more likely for products. AD uses innovative materials, such as shape memory alloys (SMAs) and shape memory polymers (SMPs), to perform a specialized release action upon application of an external field greatly limiting machine or manual labor and allowing for batch disassembly processing.[3] On the basis of past work, this paper will investigate a new approach for AD using multiple-field actuation. Multiple-field actuation will limit the probability of accidental disassembly, allow for more control in the AD process, and reduce disassembly time for AD products. The remainder of this paper will discuss the motivation for a multiple-field AD process, the materials and mechanisms for multiple-field AD, and compare the performance of this new AD process to that of a single-trigger AD process through finite element analysis.

■ BACKGROUND

SMPs and their composites are novel materials that have the ability to perform a designed shape recovery upon application of an applied environmental field. This has made SMPs useful in a number of applications, most notably as actively releasable fasteners. Past work has exhibited the usefulness of heat-releasable SMP snap-fits (see Figure 1).[3,4] In this research a SMP snap-fit was designed, manufactured, and tested for electronic product disassembly. The results from this research illustrate the feasibility of AD with the releasable snap-fits because of the limited operator or machine interference for disassembly, the generality of the design that promotes use in a variety of products, and preservation of the product integrity given proper design and application of the product. There were, however, some concerns with the research, more specifically with the single thermal trigger. In this research, the possibility of accidental disassembly of the snap-fit was lowered by choosing a SMP with a high transition temperature (105 °C). While this made it difficult for ambient or elevated temperatures to accidentally trigger the snap-fit, such a high transition temperature required a long heating cycle for disassembly,

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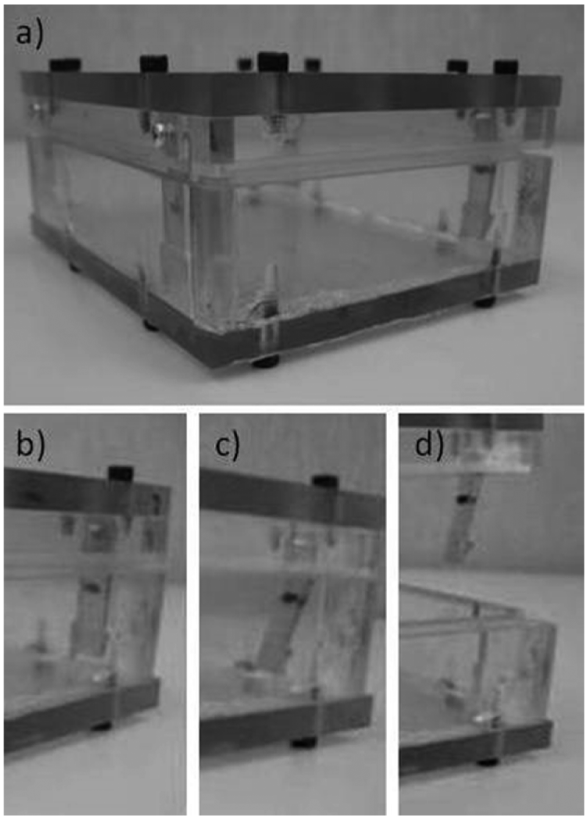

Figure 1. Disassembly process: (a) assembled housing with latched snap-fits, (b) magnified view of the engaged SMP snap-fit, (c) magnified view of the enclosed housing after heating to the transition temperature and SMP snap-fit release, and (d) magnified view of the separation of housings.

which lowered the efficiency of the disassembly process. The high transition temperature could also harm the housing or its components if special considerations were not made during design. This would especially be true for electronic products that are limited to 50−60 °C in their operation or storage temperature. Finally, the single thermal trigger does not offer many control parameters for process optimization.

On the basis of this previous work, the need for a multi-trigger element for AD becomes evident. A multi-trigger SMP composite AD element will (1) significantly limit accidental disassembly by requiring two or more unique environmental conditions for disassembly, (2) provide more control in the AD process with additional control parameters because of the multi-triggers, and (3) prevent product destruction by limiting the extreme conditions needed for single-trigger AD.

While these benefits motivate the definite need for multi-trigger AD elements, there have been no works that attempt to even conceptualize such elements because multi-trigger smart materials do not exist.[5] It has thus become the purpose of this research to create a multi-trigger smart material by the development of a shape memory polyurethane (SMPU) nanocomposite filled with nanosized magnetite particles, which is triggered by a combination of thermal and magnetic fields.

■ EXPERIMENT AND RESULTS

A SMP nanocomposite was prepared and tested by derived thermomagnetic mechanical methods, thermomechanical methods, and shape memory methods. Processing and testing provided results of an ability of the SMP nanocomposite to be controlled in shape deformation and recovery with both thermal and magnetic fields. The following sections will focus on the preparation and behavior of this material and how it was modeled for AD simulations.

SMP Nanocomposite Preparation. A commercially available SMPU (Diaplex MS5520) and magnetite nanoparticles [NanoArc, iron(III) oxide, 20−40 nm APS powder from Alfa Aesar] were used to form the SMP nanocomposite. In processing, the Diaplex resin [70 wt % *N*,*N*-dimethylformamide (DMF)/30 wt % SMPU] was vigorously blended with the desired 15 wt % portion of magnetite nanoparticles. The mixture was then poured in a mold treated with Frekote 720NC mold release and degassed for 12 h to remove air bubbles. For removal of DMF, the mold was placed in an oven at 80 °C for 48 h. The resulting sheet of SMP nanocomposite was machined to produce block samples (5 × 1 × 50 mm) for testing.

Thermomechanical Behavior. The SMP nanocomposite is based on the SMP polymer matrix. SMPs have the ability to hold and recover temporary deformations upon application of a heat field.[6,7] The basis of this ability is made through the copolymers of the matrix. The copolymers are mismatched according to their transition temperature. The "hard" segment cross-links of the matrix are created by the copolymer with the higher transition temperature, and the "switching" segments are the copolymer with the lower transition temperature. The shape memory ability of the SMP is developed through these segments. In the SMP, the "hard" segment cross-links will set and remember the permanent shape of the SMP and the "switching" segments will enable the SMP to be deformed and hold deformations in and out of the transition state.[8−10]

The addition of the nanofiller to the SMP matrix does not hinder this shape memory behavior for the SMP nanocomposite, and the same hyperelastic behavior is seen when the SMP nanocomposite is above its transition. Above the transition temperature, the hyperelastic behavior of the SMP nanocomposite is essential for the multi-trigger actuation and the special magnetically controlled deformations seen in its thermomechanical magnetic behavior.[11] The thermomechanical magnetic behavior of the SMP nanocomposite shows magnetically induced and controlled deformations when the SMP nanocomposite is above the transition temperature. Figure 2 compares this thermomechanical behavior: testing below the transition temperature (i.e., no applied heat field) shows little deformation with the applied magnetic field, and testing above the transition temperature (i.e., applied heat field) shows drastic deformation with the same magnetic field. This exhibits

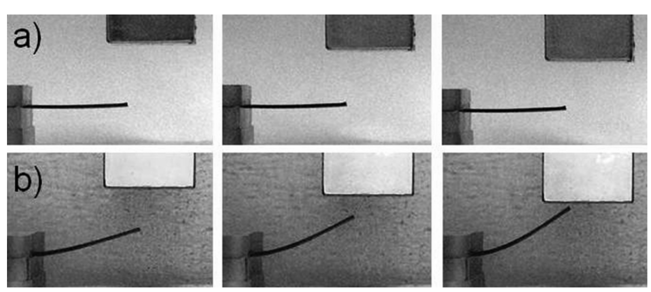

Figure 2. Comparison of magnetic effects to thermomechanical properties: (a) testing performed below the transition temperature and (b) testing performed above the transition temperature.

the desired thermomechanical magnetic behavior, where deformation of the SMP nanocomposite is made with both an applied thermal and heat field.

The quantitative difference of the effect that the applied magnetic field has on the SMPU nanocomposite above the transition temperature can be seen in Figure 3. These deflections are due to the strength and proximity of the magnet to the generally stiff sample. The stiffness of the sample is drastically decreased when above the transition, which allows for large deflections of the sample.

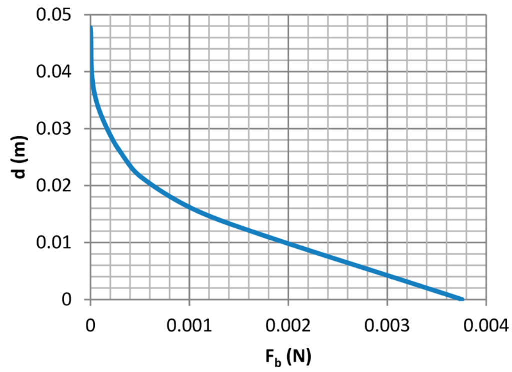

Figure 3. Results of magnetic field testing above the transition temperature.

Modeling and Simulation. The general approach for three-dimensional (3D) modeling of SMPs has been through constitutive modeling based on storage deformation,[12,13] phase transition,[14,15] and viscoelasticity.[16] The applicability of the viscoelasticity constitutive models is questionable for this work per the change in architecture of the polymer with the addition of magnetic particles and will thus be ignored. Storage deformation models and phase transition models, however, provide the needed flexibility for proper modeling of the multi-trigger composite. There are strong similarities between the two methods, because storage deformations essentially account for two phases of the SMP transition: an active phase and a frozen or storage phase. Phase transitions essentially build upon this by detailing more phases, including an initial frozen phase, a deformed frozen phase, and an active phase.

With such similarities, it is prudent to consider both for modeling as the storage deformation methodology builds upon the phase transition methodology. As an added effect, the existing SMP models will need to be compounded with an additional phase for the SMP nanocomposite in its magneto-active state. In consideration of this state, models developed for magnetoactive elastomers (MAEs) were consulted. MAEs are hyperelastic materials filled with magnetic particles. Upon application of a magnetic field, the mechanical properties change within the MAE to allow for controlled deformations. This would be very similar to the SMP nanocomposite, which exhibits a magnetically controlled deformation when heated above its transition temperature and placed in a magnetic field. The subsequent sections will establish the unique phases for the multi-trigger SMP nanocomposite and consider the constitutive model for the SMP nanocomposite.

On the basis of the knowledge gained from the constitutive models for SMPs and magnetoactive MAEs, an all inclusive model will be developed that will show the relationships for heat and magnetic SME actuation. This model will be developed on the phase transition methodology. The developed model will follow considerations similar to those for SMPs but will include additional active phases, where possible magnetic actuation is seen. The phases will be as follows. (1) Thermal active phase (AP) is seen when the SMPU nanocomposite is above T_{trans} and the transition magnetic field is absent. This field would indicate the change in material properties for the SMPU nanocomposite at elevated temperatures. As with the volume fraction modeling, the volume fraction for the SMPU nanocomposite will be denoted by f_{ta}. (2) Magnetic active phase (MAP) is seen when the SMPU nanocomposite is above T_{trans} and the transition magnetic field is present. This phase would show the necessary actuation of the SME per the two fields. The volume fraction for the SMPU nanocomposite in this phase will be denoted by f_{ma} (3) Frozen deformed phase (FDP) is seen following deformation and cooling of the SMPU nanocomposite, as with the previous model. The volume fraction of the FDP, f_T, becomes predominant when fully cooled. (4) Initial frozen phase (IFP), as with the previous model, will be the initial configuration of the SMP upon processing. This phase is predominant following heat-activated shape recovery and cooling. Its volume fraction is denoted by f_{f0}.

Similar to the frozen volume fraction, which is shared by the FDP and IFP, the active phases will also share volume fraction. Understanding the volume fractions for each phase is necessary to develop the necessary mechanical properties at a particular set of conditions. Of particular importance is the intent of the magnetic field for magnetorhelogical or magnetic deformation. The ability to which the phase relationships can be changed and, thus, the material properties of the SMPU nanocomposite will make this model useful for either case of magnetic effect.

For the SMP nanocomposite, the basis of the model will be on the phase transition model developed by Qi et al.[14] and will be the focus for the AP, FDP, and IFP phases in the model. As a means to consider the MAP phase, the MAE models developed by Dorfmann and Ogden[17] will also be discussed.

On the basis of these phases, the basic equation for total stress becomes

$$\sigma = f_{ta}\sigma_{ta} + f_{f0}\sigma_{f0} + f_T\sigma_T + f_{ma}\sigma_{ma} \tag{1}$$

where σ_{ta}, σ_{f0}, σ_T, and σ_{ma} denote the stress within the AP, FDP, IFP, and MAP, respectively. Volume fractions for the given phases are dependent upon the temperature, T. As such, the heat-transfer capability of the SMP nanocomposite must be considered. Accordingly, the temperature of the SMP nanocomposite can be modeled according to the heat transfer using Fourier's law. A simple model for the heat transfer between the heating body and the part can be calculated by determining

$$t = -T \ln \frac{T_\infty - T_{trans}}{T_\infty - T_i} \tag{2}$$

where T is a time constant for the part, T_i is the initial temperature of the part, T_∞ is the temperature of the heating body, and t is the time to heat the part to its transition temperature (T_{trans}). The time constant T will thus be dependent upon the heat-transfer coefficient between the part and the heating body via

$$T = \frac{\rho c V}{\bar{h} A} \tag{3}$$

where ρ is the density of the part, c is the specific heat capacity of the part, V is the volume of the part, $\bar{h}$ is the heat-transfer

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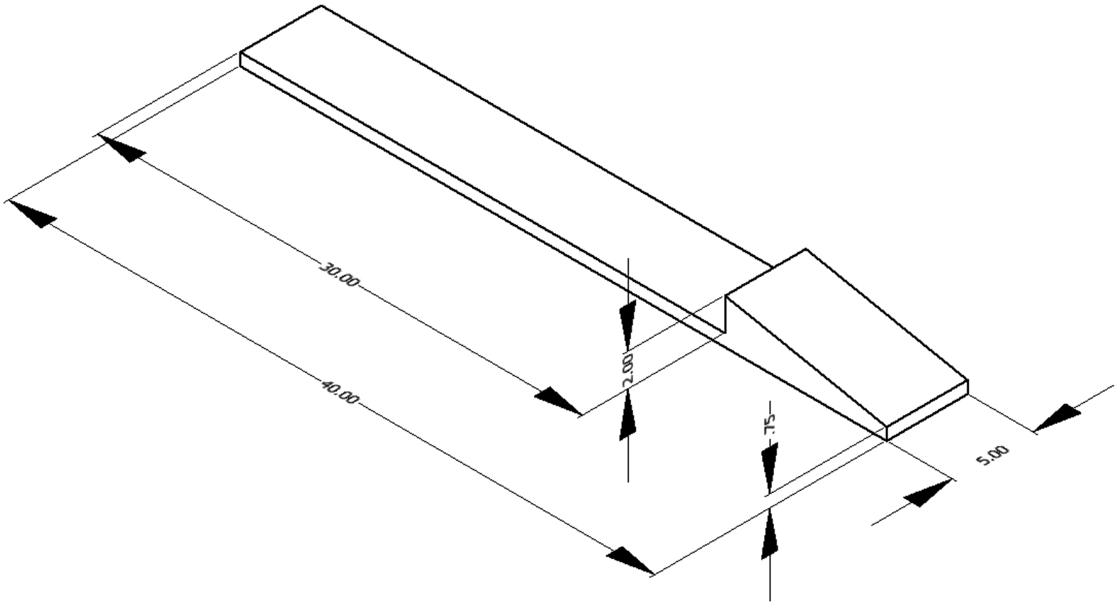

Figure 4. Snap-fit design for LS-DYNA simulation (measurements in millimeters).

coefficient between the part and the heating body, and A is the heating area of the part.[18]

There are two phases that occur above the transition temperature, AP and MAP. Because of this, f_{ta} and f_{ma} are considered jointly and are dependent upon each other. The general phase is defined as

$$f_{ta} = \frac{1}{1 + \exp\left[-\frac{T - T_r}{B}\right]} \tag{4}$$

where T_r is the reference temperature close to T_{trans} and B is the parameter that characterizes the transition zone. Considering the purely thermal effects of the AP phase, the MAP is dependent upon this phase when in the presence of the magnetic field. Therefore, the AP and MAP phases are inversely proportional. When the SMP nanocomposite is in the presence of a magnetic field, $f_{ma} = 1$ and $f_{ta} = 0$. Conversely, when above the transition temperature and in the absence of a magnetic field, $f_{ma} = 0$ and $f_{ta} = 1$.

Taking the volume fraction of the active phase (both thermally active and magnetically active) and subtracting it from one will give the volume fraction of the frozen phase. Because the frozen phase is then determined by the relationship between FDP and IDP, it becomes necessary to distinguish what frozen phase the SMP nanocomposite is in at a given time, t. At initial conditions, where the SMP is in its permanent shape and below T_{trans}, the volume fraction follows:

$$f_{f0}|_{t=0} = f_f|_{t=0} \qquad f_T|_{t=0} = 0 \tag{5}$$

Upon thermal loading, deformation, and cooling, this frozen phase will create a change in the frozen configuration from the initial rigid configuration to the deformed rigid configuration. Likewise, upon thermal loading and shape recovery, the frozen configuration will show the same change from the deformed rigid configuration to the initial rigid configuration. This change in the frozen volume is thus denoted by Δf_f. Accordingly

$$f_{f0}|_{t=0} = f_f|_{t=0} \qquad f_T|_{t=2} = f_T|_{t=1} + \Delta f_f \tag{6}$$

$$\Delta f_{f0} = \frac{f_{f0}}{f_{f0} + f_T}\Delta f_f \qquad \Delta f_T = \frac{f_T}{f_{f0} + f_T}\Delta f_f \tag{7}$$

where Δf_{f0} is the volume fraction from the IFP and Δf_T is the volume fraction from the FDP.

LS-DYNA FEA Simulation. The subsequent sections will further the analysis of this chapter and will provide simulation analysis for the application of AD. The focus of this additional content will be on the design and simulation of a SMP and SMP nanocomposite snap-fit. As part of this analysis, the material properties and thermal properties of the tested Diaplex SMP nanocomposite will be used in the simulation of a multi-trigger snap-fit. For the single-trigger snap-fit simulation, a hypothetical SMP will be used with the same mechanical and thermal properties of the Diaplex SMP nanocomposite, with the exception of the transition temperature. For the SMP snap-fit, the T_{trans} of 105 °C will instead be 55 °C. This increase in transition temperature is assumed as a means to reduce the possibility of accidental disassembly. The multi-trigger disassembly mechanism of the SMP nanocomposite allows for the manufacturer-defined 55 °C.

The same snap-fit design was used for the analysis of both the SMP heat-releasable fastener and the SMP nanocomposite. The design of the snap-fit is a basic 40 mm beam with a 10 mm long and 2 mm high fastening section (see Figure 4). As part of the simulation, it is assumed that the 10 mm non-fastening section of the snap-fit is fixed. This is performed for both cases and is needed to hold the snap-fit within the assembly for shape recovery and deformation for release.

LS-DYNA simulations considered the processes to reach the disassembly for both the SMP and SMP nanocomposite snap-fit. For the SMP snap-fit, the disassembly state is reached when the trained snap-fit is heated from room temperature (25 °C) above its T_{trans} (105 °C with a ±5 °C transition zone). The high transition temperature for the SMP is justified because 105 °C would most likely never be seen in elevated ambient conditions, making a case of accidental disassembly highly unlikely. The SMP snap-fit simulation will thus need to consider a training process that would straighten it for assembly along with this disassembly process. In the training process, the snap-fit will be heated above T_{trans} and deformed to a straight assembly state. The same thermal parameters will be assumed in this training process. In heating for shape recovery and training for the SMP snap-fit, an oil bath at 125 °C will be used for the simulation. Similarly, for the SMP nanocomposite snap-fit, an oil bath at 75 °C will be used. Also, for the SMP nanocomposite snap-fit, the disassembly state will be reached when the snap-fit is heated from room temperature above its T_{trans} (55 °C with a ±5 °C transition zone) and a magnetic field is applied for mechanical deformation.

The disassembly state for the SMP snap-fit is solely dependent upon the applied thermal field. The same shape recovery approach with the produced simulation models will thus be used to show the through temperature-dependent prescribed motion boundary condition. This prescribed motion curve will relate to the time/temperature that it takes the snap-fit to reach the 2 mm needed for release. The disassembly state for the SMP nanocomposite is dependent upon both an applied thermal field and a magnetic field. The simulation to reach this disassembly state will thus show the heating of the SMP nanocomposite to 60 °C (the end of the transition zone), at which point the magnetic field will be applied. Because the design of the SMP nanocomposite is so similar to the tested and simulated SMP nanocomposite beam, it is assumed that the same magnetically controlled deformation will be seen. The same correlated mechanical load will thus be applied to the SMP nanocomposite snap-fit for disassembly. As with the SMP snap-fit, the time at which the SMP nanocomposite reaches the 2 mm needed for release will be the disassembly time.

Simulation Results. The disassembly simulation for the SMP nanocomposite is seen in Figure 5. The results from this simulation correlate a mechanical load to a magnetic force for the SMP nanocomposite, causing the needed deflection of the SMP nanocomposite snap-fit for release at its T_{trans}. The time for disassembly is the heat time to transition (approximately 6.7 s), and the applied magnetic field (approximately 0.3 s) results in an approximate 7 s disassembly time.

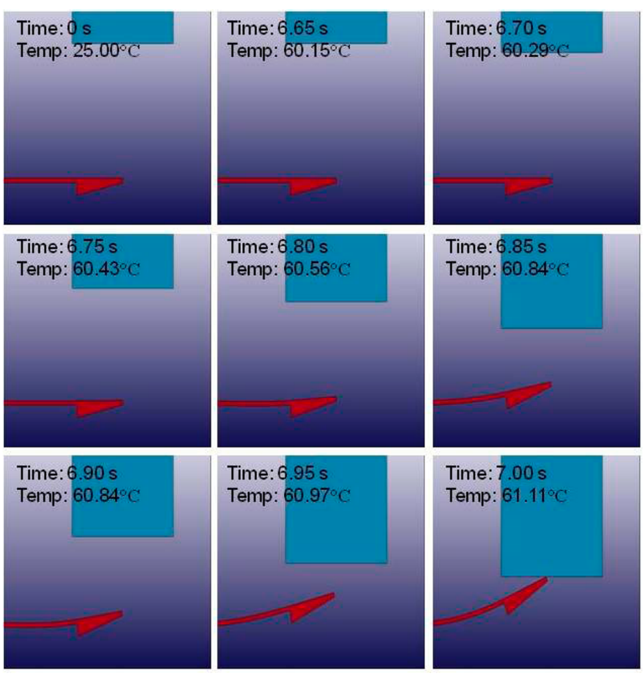

Figure 5. LS-DYNA simulation results for SMP nanocomposite snap-fit.

The training process and disassembly process were both simulated for the SMP snap-fit. The training process is needed to straighten the snap-fit for assembly and use. The time to train the snap-fit is dependent upon the time that it takes to heat the snap-fit above its transition, deform it, and cool it while holding the deformation. For the simulation, the training process considers the time to heat (approximately 9 s) and apply a mechanical force to deform (approximately 1 s). Quenching the snap-fit would rapidly set the deformation of the snap-fit to complete the training process and, thus, can be ignored because it would make a small portion of the total training time of 10 s.

The disassembly results for the SMP snap-fit are seen in Figure 6. The disassembly process is based on the shape memory recovery that is determined by the temperature of the snap-fit. On the basis of the simulation parameters, the SMP snap-fit would totally recover its shape in approximately 10 s and would reach the needed 2 mm for disassembly in approximately 9 s.

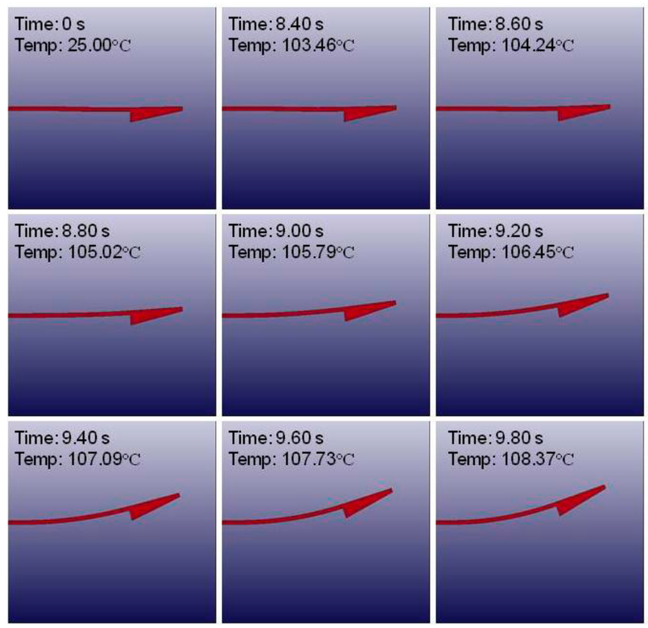

Figure 6. LS-DYNA simulation result for SMP snap-fit.

■ DISCUSSION

A definite case for the SMP nanocomposite snap-fit is used over the SMP snap-fit per a shorter release time through simulation results. On the basis of the simulation conditions, the SMP nanocomposite can be released in approximately 7 s, which is 2 s shorter than the SMP snap-fit (see Figure 7). While this time may not be worthwhile in considering the need to apply a magnetic field, it should be noted that further reduction in release time for the SMP nanocomposite can be achieved when considering the temperature of the oil bath for heating. Also, for this simulation, the SMP and SMP nanocomposite share the same thermal properties (except in T_{trans}). In actuality, these materials would not share the same thermal characteristics. Specific heat capacity, heat-transfer coefficients, and thermal time constants are varied between the SMP and SMP nanocomposite, especially with a SMP with such a high

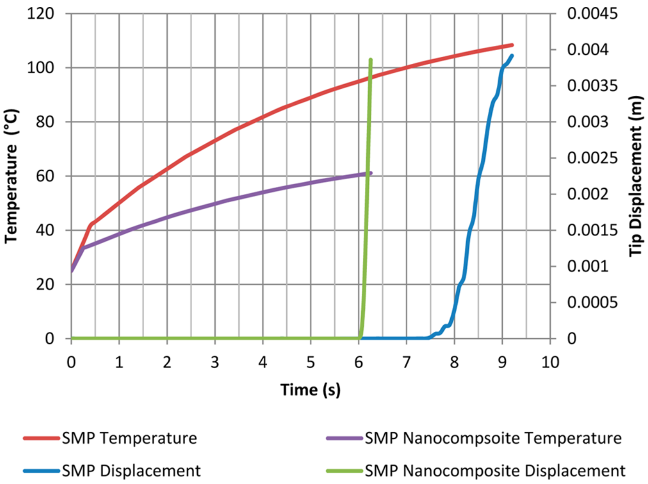

Figure 7. Snap-fit displacement and temperature with respect to time.

transition temperature. In this respect, this disassembly simulation and the parameters used provide a worst-case scenario for the SMP nanocomposite, which still shows a shorter disassembly time.

The argument for the SMP nanocomposite use in the application of AD is also encouraged by the lack of a training process (see Table 1). The training process essentially doubles the processing for the SMP snap-fit because it must be heated 2 times (once for training and once for disassembly). The SMP nanocomposite snap-fit on the other hand does not need to be trained and only needs to be heated once for disassembly.

Table 1. Total Time Difference for Processing SMP and SMP Nanocomposite Snap-Fits

material	training process time (s)	disassembly process time (s)	total
SMP	10	9	19
SMP nanocomposite	0	7	7

Another point of emphasis is the lower T_{trans}, which can be afforded to the multi-trigger snap-fit because the heat and magnetic trigger must act in tandem. If only a heat field is applied that brings the SMP nanocomposite above T_{trans}, the snap-fit will not deform, unlike the single-trigger snap-fit, which will go through its shape memory effect. Likewise, the multi-trigger snap-fit will not be affected with application of the magnetic field. For proper disassembly of the multi-trigger snap-fit, the SMP nanocomposite (1) must be brought into a transition state through an applied heat field by heating above T_{trans} and (2) cause deformation of the snap-fit for disassembly through the applied magnetic field. Furthermore, with the multi-trigger snap-fit, more control of the disassembly process is realized. Snap-fits may be strategically released upon application of both fields, allowing for step-by-step disassembly of subassemblies and components from a product. This would be similar to single-trigger actuation of fasteners with different T_{trans}.[19]

While the multiple-field release of the SMP nanocomposite snap-fit outperforms the single-field release of the SMP snap-fit, there are some design concerns for actual product implication. This would be in the specific placement of the multi-trigger snap-fits within the product and the magnitude and direction of the applied magnetic field. If not placed properly or if the magnetic field is not directed correctly, the snap-fits could not perform the needed deflection for release. This issue is not a problem with single-field actuation of the SMP snap-fit.

Ignoring the possible product design concerns with the multi-trigger snap-fit, the technical merit for this research can create a number of opportunities. The fabrication of a multi-trigger smart material will provide new avenues for the application and implementation of smart materials. The implementation of multi-trigger smart materials can change a number of designs fit for functional materials. Along with these designs, methodologies may change to appropriately apply such materials in products and applications. This would be especially true for designing products for smart disassembly. New multi-trigger releasable fasteners, as the ones presented with the research, will change the current design for disassembly methodologies and create a more efficient disassembly process for a number of products, including small electronic devices that are typically difficult and expensive to disassemble. As previously discussed, current disassembly methods fail to promote efficient and flexible disassembly, thus making disassembly an unpopular EoL activity. Past research has developed a means for making disassembly a more efficient and flexible process with AD, but with the probability of accidental disassembly because of single-trigger designs, AD has not become a widely accepted disassembly option. The proposed work for developing multi-trigger designs in this project will solve this problem and make AD an acceptable EoL activity for industry.

Further, the validity of the multi-trigger snap-fit design has been shown through thermomechanical and magnetic testing of the SMP nanocomposite, which allowed for multi-trigger disassembly simulation. More work must be performed through implementation of such devices in test products. This implementation would provide further validation of the multi-trigger fasteners and would give practical examples of certain benefits, such as thermal and magnetic sensitivities, disassembly performance, and special processing. Future experiments should also investigate more applicable SMPs for commercialization. The studied Diaplex SMP nanocomposite provided the key functionalities to exhibit the multi-trigger disassembly mechanism but is not a typical material used by current electronic manufacturers. Poly(methyl methacrylate) (PMMA) and acrylonitrile butadiene styrene/polycarbonate (ABS/PC) are more commonly used in electronic products and have exhibited shape memory properties.[20,21] With dispersion of nanomaterials, such as the magnetite as in this research, within these standard engineering materials and with their shape memory functionalities, it would be possible for experiments to be performed to show electronic manufacturers adoptable materials and designs for AD adoption.

As previously discussed, current disassembly methods fail to promote efficient and flexible disassembly, thus making disassembly an unpopular EoL activity. Past research has developed a means for making disassembly a more efficient and flexible process with AD, but with the probability of accidental disassembly because of single-trigger designs, AD has not become a widely accepted disassembly option. This work has developed a multi-trigger designs to solve this problem and make AD an acceptable EoL activity for industry. Multi-trigger AD will increase EoL product disassembly. Increased product disassembly will increase both reuse of product components and recycling of the product, which, in turn, will provide for more sustainability in product manufacturing.[1]

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Notes

The authors declare no competing financial interest.

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