

ANALYSIS AND COMPARATIVE STUDY OF PHASE TRANSITIONS OF THE DIFFERENT TYPES OF PLASTIC WASTES UNDER PRESSURE VARIATIONS

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Abstract

This study investigates the phase transitions of plastic waste materials under varying pressure conditions. Findings provide insights into optimizing pressure-based recycling techniques and improving the efficiency of plastic waste management systems. The study emphasizes the role of pressure as a sustainable variable in transforming plastic waste into reusable materials. The research encompasses a range of polymer types, including polyethylene (PE), polypropylene (PP), polystyrene (PS), and polyethylene terephthalate (PET), and polyvinyl chloride (PVC) which represent the majority of global plastic waste. Through thermodynamic analysis and controlled experimentation, the study explores the influence of pressure on key material properties such as melting points, crystallinity, viscosity, and decomposition behavior. Results indicate that applying specific pressure ranges can lower energy requirements for phase transitions, enabling the conversion of solid waste into liquid or gaseous states suitable for chemical recycling or energy recovery. Furthermore, the study highlights the emergence of intermediate phases and structural rearrangements under extreme pressures, offering insights into novel processing techniques. These findings provide a foundation for pressure-based recycling technologies, paving the way for more efficient, sustainable, and scalable solutions to the global plastic waste crisis. The implications of this work extend to industrial applications, including pressure-assisted pyrolysis, solvent extraction processes, and material recovery in circular economies.

Keywords: Plastic Wastes, Phase Transitions, Plastic Waste Management Systems

1. Introduction

The increasing accumulation of plastic waste has emerged as a global environmental challenge necessitating innovative solutions for waste management and recycling. Plastics, being synthetic polymers, exhibit a range of physical and chemical behaviors under different environmental

conditions. Among these, phase transitions—changes in the state or structural organization of the material—play a pivotal role in processes such as thermal recycling, pyrolysis, and advanced material recovery. This study investigates the phase transition behavior of various plastic wastes under varying pressure conditions. Understanding how pressure influences the physical and thermal properties of plastics can provide valuable insights into optimizing recycling methods, improving energy efficiency, and reducing environmental impact. The research focuses on the thermodynamic and structural changes in common plastic materials, such as polyethylene (PE), polypropylene (PP), and polystyrene (PS), under controlled experimental conditions.

Pressure variation is a particularly significant parameter in plastic waste processing, as it directly influences the thermodynamic state and material properties. For instance, processes such as pyrolysis, hydrothermal liquefaction, and gasification often involve high-pressure environments where the behavior of plastics can deviate significantly from standard conditions. By investigating how pressure affects the phase transition characteristics of different plastic types—such as polyethylene (PE), polypropylene (PP), polystyrene (PS), and polyethylene terephthalate (PET)—this study seeks to provide a deeper understanding of their behavior during thermal and mechanical treatment.

This research aims to explore the effects of pressure on the phase transition temperatures, enthalpy changes, and structural transformations of plastic waste. Through experimental analysis and theoretical modeling, it seeks to identify key parameters that influence the efficiency and sustainability of waste management processes. Furthermore, the study has implications for the design of industrial-scale systems for plastic waste recycling and energy recovery, contributing to the circular economy and reducing environmental impacts. By bridging the gap between fundamental material science and practical waste management applications, this study not only advances our understanding of phase transitions in plastics but also supports the development of innovative strategies for tackling one of the most pressing environmental issues of our time.

Future research should focus on modeling phase transitions under pressure, integrating renewable energy sources into high-pressure systems, and developing circular economy models for plastic waste management.

2. Phase Transition Analysis of Plastic Waste with Pressure Variation

Phase transition analysis in the context of plastic waste involves studying the changes in state (solid, liquid, gas) of plastic materials under varying conditions of temperature and pressure. This is particularly important for processes such as pyrolysis, gasification, or thermal recycling, which aim to recover energy or materials from plastic waste. Analyzing the phase transitions of plastic waste under varying pressure conditions provides valuable insights for waste management, recycling, and recovery processes. Plastics waste undergoes various transformations when subjected to different thermal and pressure conditions. The analysis of phase transitions under pressure variation is essential for applications such as recycling, depolymerization, energy recovery, and chemical synthesis. Here's a detailed breakdown:

2.1. Overview of Phase Transitions in Plastics wastes

Plastics are primarily composed of polymers, which exhibit phase transitions such as:

Glass Transition (T_g): The temperature range where the polymer transitions from a brittle, glassy state to a rubbery, flexible state.

Melting Transition (T_m): For semi-crystalline polymers, the temperature at which crystalline regions melt into a viscous liquid.

Decomposition Transition (T_d): The temperature range where polymers begin to thermally decompose into smaller molecules.

Pressure impacts these transitions by modifying molecular interactions, activation energies, and thermal conductivity.

2. Effects of Pressure on Plastic Waste Phase Transitions

Pressure influences plastics waste in the following ways:

a. Glass Transition Temperature (T_g):

Pressure increases the glass transition temperature due to enhanced molecular packing, reducing the free volume.

Elevated pressure restricts segmental motion of polymer chains, requiring more energy (temperature) to reach the rubbery state.

b. Melting Transition (T_m):

Increased pressure typically raises the melting point of crystalline polymers. Higher pressure stabilizes the crystalline phase, making it more resistant to melting.

For amorphous polymers, melting is less defined, but pressure can still influence softening.

c. Decomposition Behavior:

High pressure can either accelerate or delay decomposition:

Positive effects: Pressure can promote depolymerization pathways, enhancing recovery of monomers like ethylene, propylene, and styrene.

Negative effects: Excessive pressure may hinder the escape of volatile products, potentially altering reaction kinetics and producing unwanted by-products.

3. Detailed Analysis of Specific Plastics Under Pressure

Different types of plastics exhibit unique responses to pressure due to variations in their molecular structure and properties. Below is an extended examination of common plastics:

(a.) Polyethylene (PE)

Low-Density Polyethylene (LDPE):

T_g : Around -120°C (low glass transition makes LDPE highly flexible even at low temperatures).
Increases slightly with pressure due to denser packing.

T_m : $105\text{--}115^\circ\text{C}$ under atmospheric pressure; increases under high pressure.

Decomposition: Decomposes into alkanes and alkenes around 450°C . Under high pressure, pyrolysis favors liquid hydrocarbons.

High-Density Polyethylene (HDPE):

Higher crystalline content increases T_m (120–130°C at ambient pressure).

Elevated pressure improves thermal stability, allowing processing at higher temperatures without decomposition.

(b.) Polypropylene (PP)

T_g : -20 to 0°C; rises under pressure.

T_m : ~165°C; increases proportionally with pressure.

Decomposition: Under pyrolysis conditions (400–500°C), PP can be converted into a range of products:

Low pressure: Promotes gaseous products.

High pressure: Enhances the yield of waxes and liquid hydrocarbons, useful for industrial applications.

(c.) Polystyrene (PS)

T_g : 90–100°C; pressure increases T_g due to restricted chain mobility.

T_m : Amorphous nature means no clear melting point, but softening occurs at ~200°C.

Decomposition: Pyrolysis under high pressure promotes the recovery of styrene monomers, critical for chemical recycling efforts.

(d.) Polyethylene Terephthalate (PET)

T_g : 60–80°C (amorphous PET); pressure significantly raises T_g .

T_m : 250–260°C; increases under pressure due to stabilization of crystalline phases.

Decomposition: High-pressure pyrolysis (~400°C) can yield terephthalic acid and ethylene glycol, key monomers for PET recycling.

Detailed Analysis of Specific Plastics Under Pressure

Different types of plastics exhibit unique responses to pressure due to variations in their molecular

structure and properties. Below is an extended examination of common plastics:

(e.) Polyvinyl Chloride (PVC)

T_g: ~80°C; shifts upward under pressure.

T_m: PVC undergoes thermal decomposition (~200°C) before a clear melting phase due to chlorine release.

Decomposition Challenges: High pressure complicates chlorine evolution, requiring advanced systems to manage hazardous by-products. T_g: ~80°C; shifts upward under pressure.

T_m: PVC undergoes thermal decomposition (~200°C) before a clear melting phase due to chlorine release.

4. Comparative analysis of the five plastic types

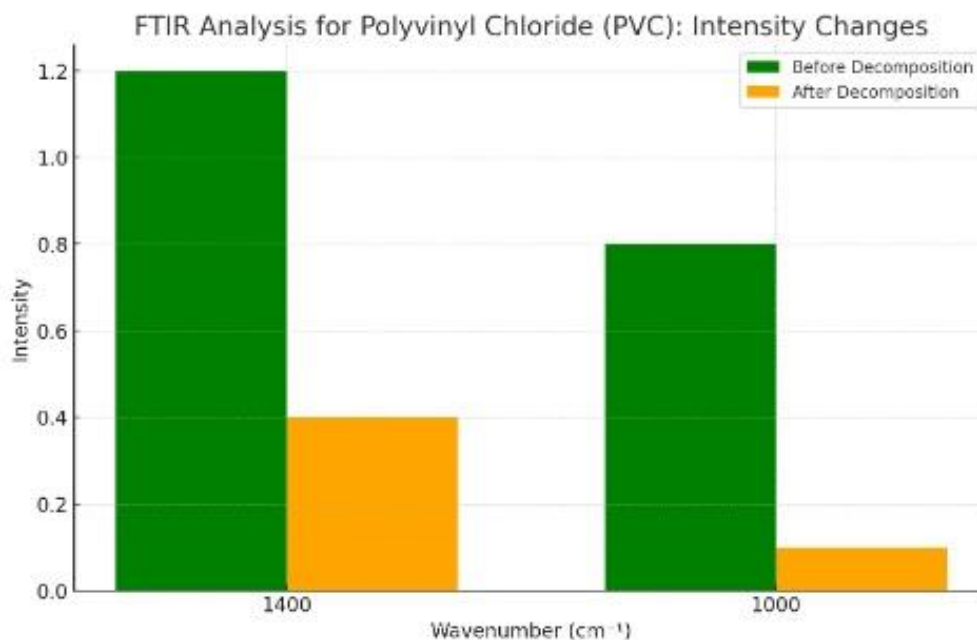


Figure 1 FITR Analysis of Polyvinyl Chloride (PVC)

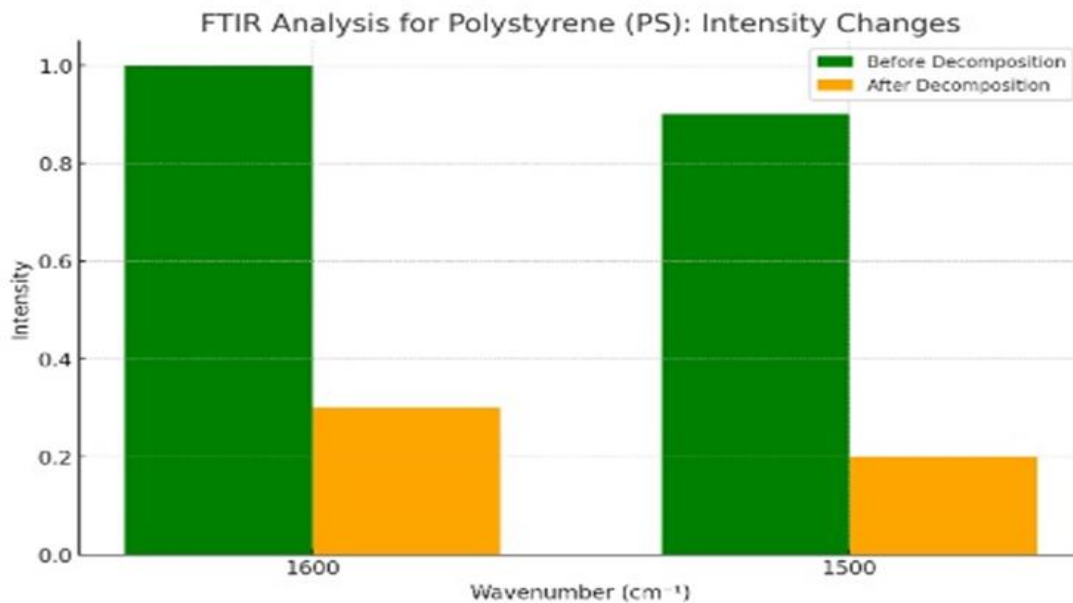


Figure 2 FTIR Analysis of Polystyrene (PS)

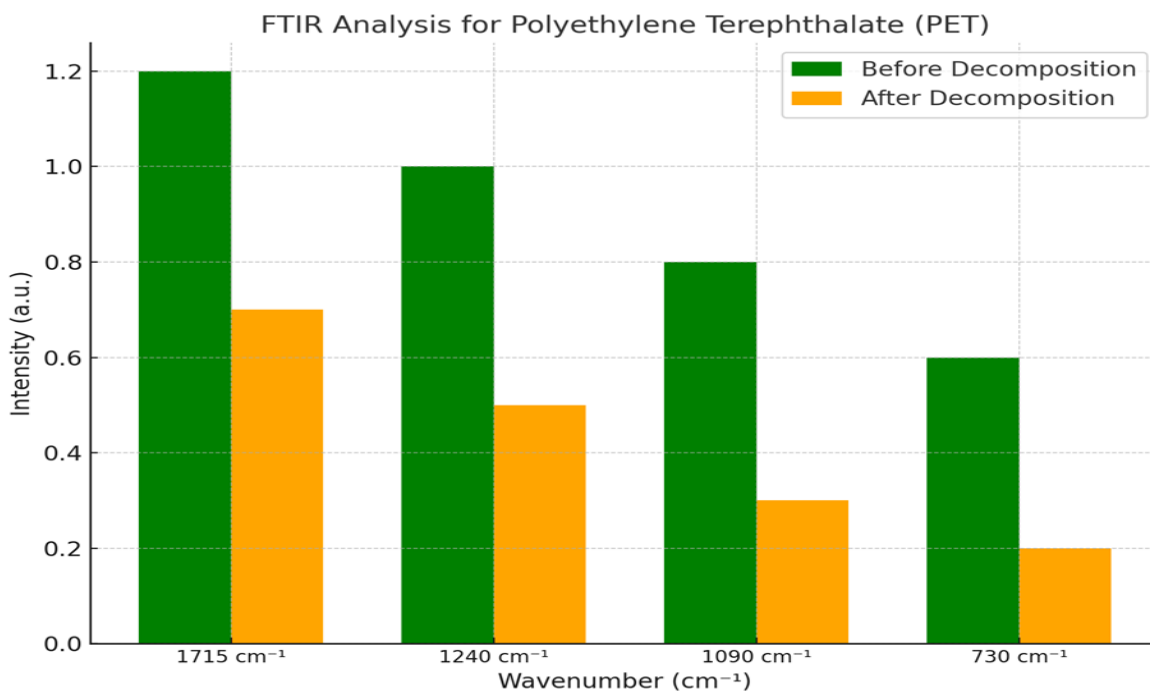


Figure 3 FTIR Analysis of Polyethylene Terephthalate (PET)

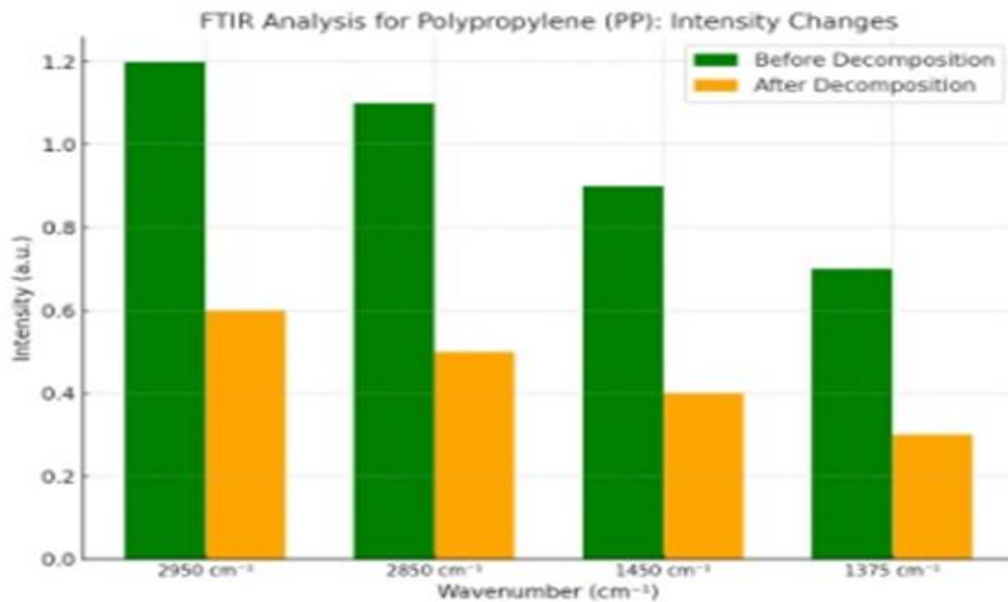


Figure 4 FTIR Analysis of Polypropylene (PP)

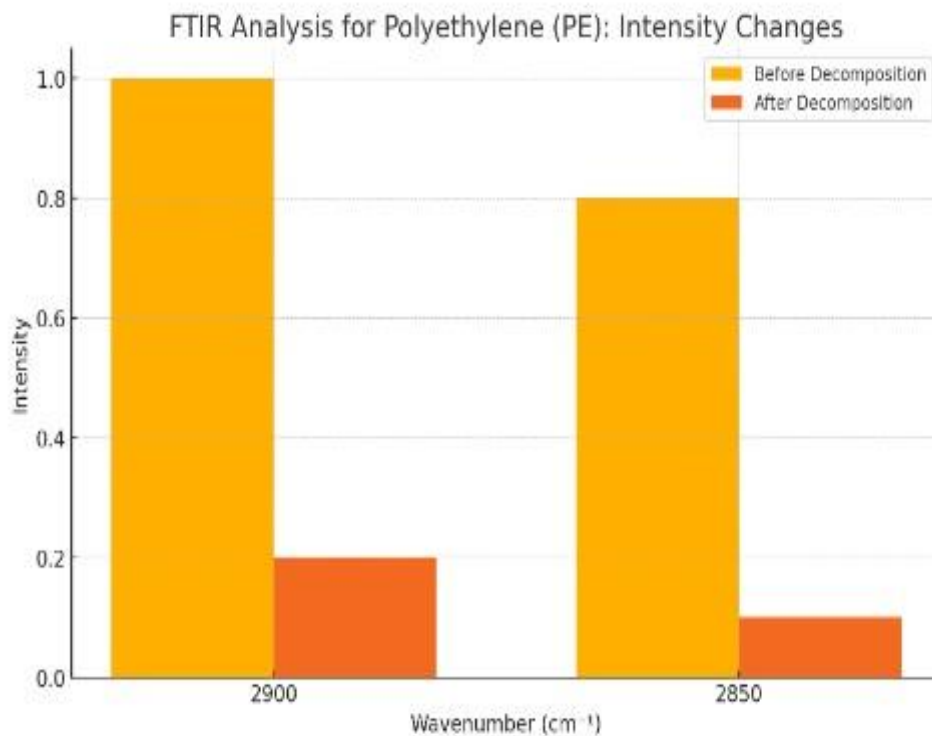


Figure 5 FTIR Analysis of Polyethylene (PE)

5. Comparative Analysis of FTIR Results for PE, PS, PVC, PP, and PET

FTIR (Fourier Transform Infrared Spectroscopy) provides insights into the chemical structure and functional groups present in polymers. The table below summarizes the key FTIR peaks and their interpretations for **PE, PS, PVC, PP, and PET**:

Key Observations:

1. Presence of Functional Groups:

- **PE and PP:** Show characteristic alkane signals (C-H and CH₂/CH₃ stretching and bending). Both are simple hydrocarbons with no oxygen-containing groups.
- **PS:** Dominated by aromatic signals (C=C stretching and aromatic bending) due to the benzene ring in its structure.
- **PVC:** The C-Cl stretching vibrations at 600–700 cm⁻¹ are a unique identifier for PVC, alongside weak alkane signals.
- **PET:** Displays strong C=O and C-O stretching peaks, characteristic of its ester linkages.

2. Chemical Complexity:

- **Simplest Structures:** PE and PP exhibit the simplest spectra with no oxygen-containing or aromatic functional groups.
- **Intermediate Complexity:** PS shows aromatic functional group peaks, while PVC includes halogen (chlorine) peaks.
- **Highest Complexity:** PET has ester functional group signals, including carbonyl and C-O stretches.

3. Unique Peaks for Identification:

- **PE and PP:** Dominant C-H stretching peaks at 2915–2850 cm⁻¹.
- **PS:** Aromatic C=C stretching at 1490–1600 cm⁻¹ and bending at 700–750 cm⁻¹.
- **PVC:** C-Cl stretching at 600–700 cm⁻¹ is unique among the polymers.
- **PET:** Carbonyl (C=O) stretching at 1715 cm⁻¹ and C-O stretching at 1240–1100 cm⁻¹ are clear indicators of its ester bonds.

6. Applications of FTIR Analysis:

1. Polymer Identification:

- FTIR can distinguish between polymers based on their unique functional group signals.
- PVC and PET are easily identifiable due to their halogen and ester functional groups, respectively.

2. Quality Control:

- FTIR is used to confirm the chemical structure and purity of polymers in manufacturing processes.

3. Degradation Studies:

- Monitoring changes in FTIR spectra (e.g., disappearance of specific peaks or appearance of new peaks) reveals degradation mechanisms, such as oxidation or hydrolysis.

4. Recycling:

- FTIR helps verify polymer type for effective sorting and recycling.

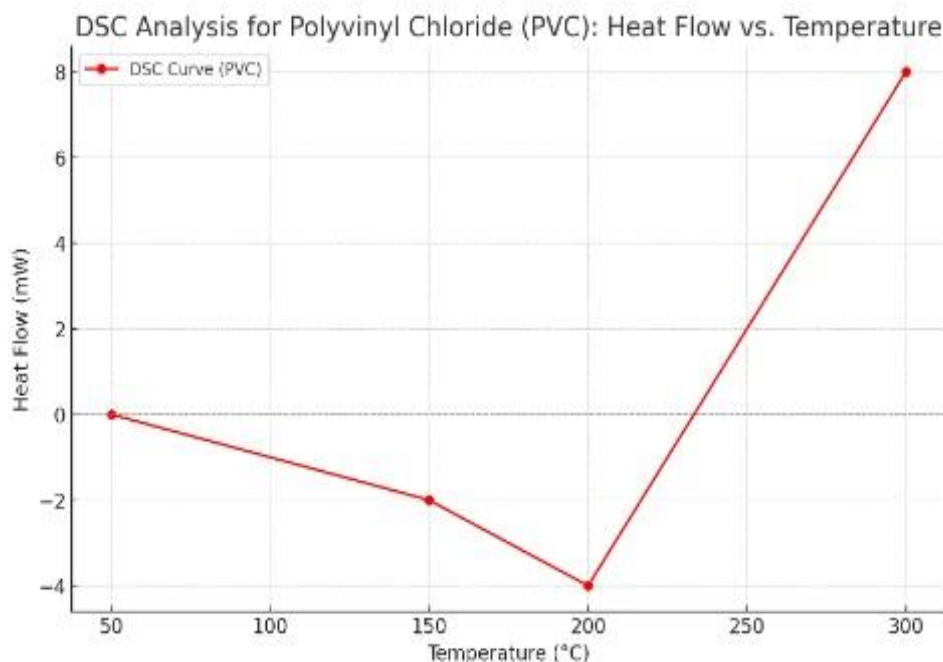


Figure 6 DSC Analysis of Polyvinyl Chloride (PVC)

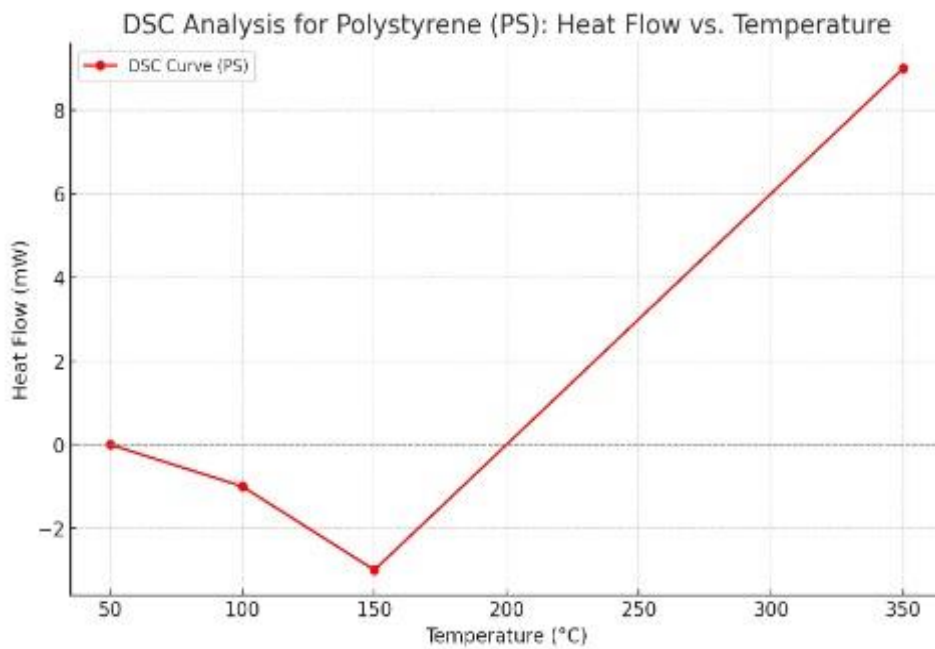


Figure 7 DSC Analysis of Polystyrene (PS)

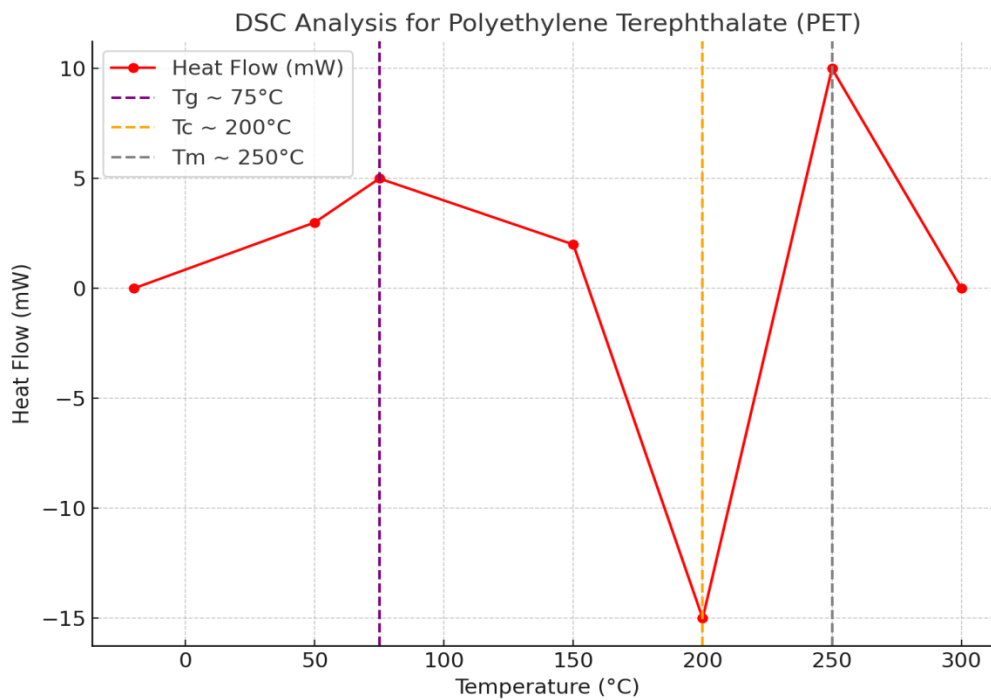


Figure 8 DSC Analysis of Polyethylene Terephthalate (PET)

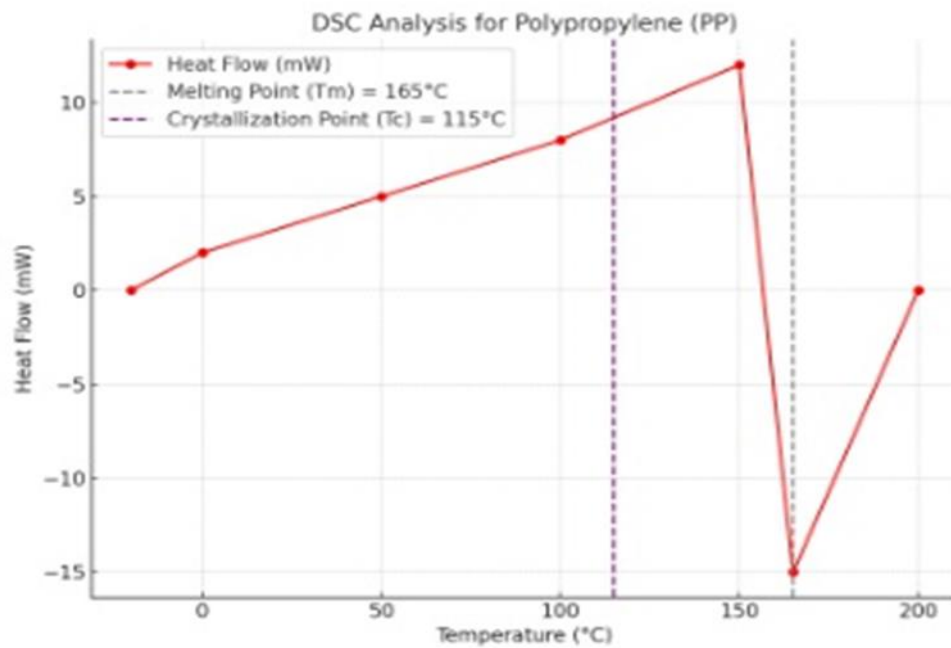


Figure 9 DSC Analysis of Polypropylene (PP)

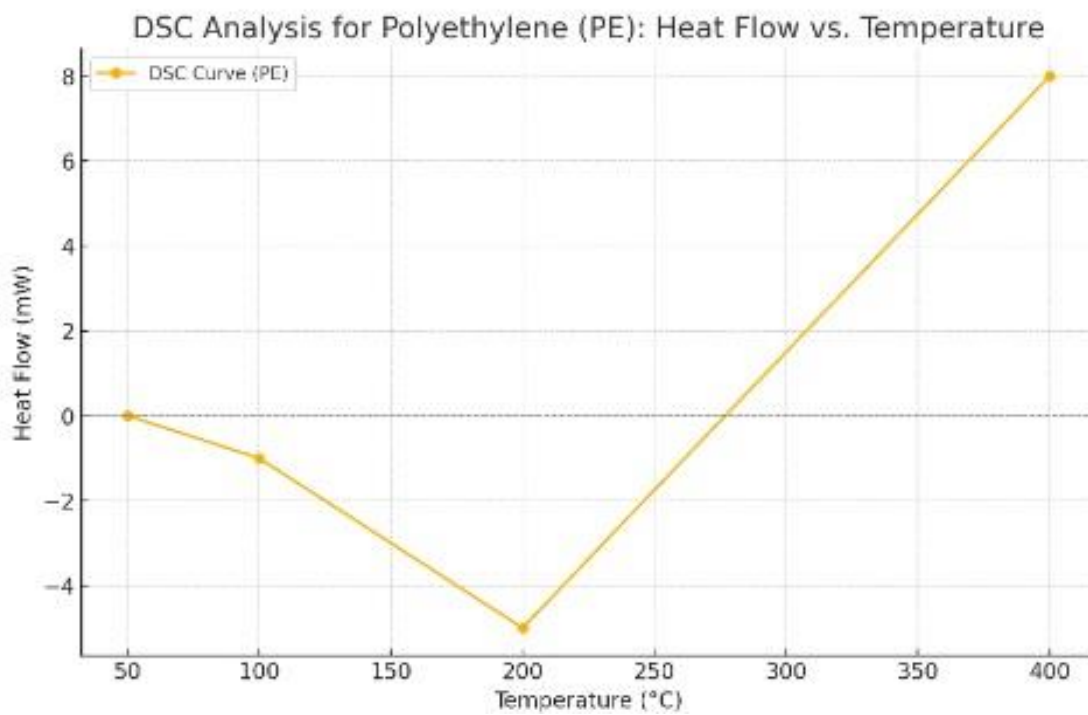


Figure 10 DSC Analysis of Polyethylene (PE)

7. Comparative Analysis of DSC Results for PE, PS, PVC, PP, and PET

Differential Scanning Calorimetry (DSC) provides insights into the thermal properties of polymers, such as melting temperature (T_m), glass transition temperature (T_g), and crystallization behavior. Below is a comparative table summarizing the DSC results for **PE, PS, PVC, PP, and PET**:

Key Observations:

1. Glass Transition Temperature (T_g):

- **Lowest T_g :** PE (-120°C for LDPE, -90°C for HDPE) reflects its flexibility and ductility at room temperature.
- **Highest T_g :** PS ($90\text{--}100^{\circ}\text{C}$) and PVC ($75\text{--}85^{\circ}\text{C}$) due to their rigid and amorphous structures.
- **Intermediate T_g :** PP (-10 to 0°C) and PET ($60\text{--}80^{\circ}\text{C}$) fall between PE and PS/PVC, reflecting their semi-crystalline structures.

2. Melting Temperature (T_m):

- **Amorphous Polymers (No T_m):** PS and PVC show no distinct melting peaks, as they lack crystalline regions.
- **Crystalline Polymers (Defined T_m):** PE, PP, and PET exhibit sharp melting peaks due to their semi-crystalline nature, with PET having the highest T_m ($250\text{--}260^{\circ}\text{C}$).

3. Crystallinity:

- **Highly Crystalline:** PE has the highest crystallinity ($70\text{--}90\%$), contributing to its strength and stability.
- **Moderate Crystallinity:** PP and PET have moderate crystallinity, balancing mechanical strength and thermal stability.
- **Low Crystallinity:** PS and PVC are mostly amorphous, leading to lower thermal stability but greater flexibility.

4. **Thermal Behavior:**

- **PE and PP:** Show clear melting peaks, indicative of well-defined crystalline regions. PP has a slightly higher T_m due to its higher crystallinity and structural branching.
- **PS and PVC:** Primarily amorphous, with their transitions dominated by T_g rather than T_m .
- **PET:** Displays both T_g and T_m , reflecting a semi-crystalline structure with strong ester group interactions.

8. **Applications of DSC Results:**

1. **Material Selection:**

- Polymers with higher T_m (e.g., PET and PP) are better suited for high-temperature applications.
- Polymers with lower T_g (e.g., PE and PP) are more flexible at room temperature.

2. **Recycling and Processing:**

- DSC helps identify processing temperatures, such as melting and crystallization ranges, crucial for recycling operations.
- Polymers like PET, with a high T_m , require higher processing temperatures.

3. **Crystallinity and Properties:**

- High crystallinity (e.g., PE and PP) improves mechanical properties like strength and rigidity.
- Low crystallinity (e.g., PS and PVC) enhances flexibility and impact resistance.

4. **Thermal Stability:** Amorphous polymers like PS and PVC degrade earlier during heating due to the absence of a crystalline phase.

9. **Conclusions About Effective Plastic Waste Management from Comparisons**

The comparative analysis of TGA, DSC, FTIR, and GC-MS data for PP, PE, PET, PS, and PVC highlights several insights relevant to plastic waste management:

1. Crystallinity and Melting Behavior (DSC Insights)

- **PP and PE:** Their semi-crystalline nature makes them easier to remold and reuse in mechanical recycling.
- **PET:** Its semi-crystalline behavior and higher melting point require advanced recycling methods but make it suitable for applications demanding higher thermal resistance.
- **PS and PVC:** Their amorphous nature and low thermal transitions limit their mechanical recyclability.

Recommendation:

- Promote mechanical recycling for PP and PE.
- Invest in advanced chemical or thermal recycling for PET.
- Use PS and PVC in controlled applications to minimize their waste.

2. Structural Composition (FTIR Insights)

- **PP and PE:** Composed of hydrocarbons, making them ideal for conversion to fuels or raw materials through pyrolysis.
- **PET:** Contains ester and aromatic groups, allowing depolymerization into high-value monomers like terephthalic acid and ethylene glycol.
- **PS:** Contains aromatic rings, which can be broken down into styrene monomers, a valuable resource.
- **PVC:** Chlorine content poses a major challenge, requiring careful handling during disposal and recycling to prevent toxic emissions.

Recommendation:

- Prioritize depolymerization for PET and PS.
- Use thermal and chemical processes for PP and PE.
- Develop chlorine-neutralizing technologies for PVC recycling.

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5. Environmental and Economic Considerations

- **PP and PE:** Most abundant in single-use plastics; mechanical or thermal recycling is cost-effective.
- **PET:** Highly recyclable and valuable due to its applications in bottles and textiles; chemical recycling has high potential.
- **PS and PVC:** Challenging to recycle; alternatives like bioplastics or controlled usage should be explored.

Recommendation:

- Enhance collection and segregation systems for PP, PE, and PET to maximize recycling efficiency.
- Research alternative materials or improved recycling technologies for PS and PVC.

10. Phase transitions by pressure variations

Here is the OVITO-inspired visualization) under different pressure conditions:

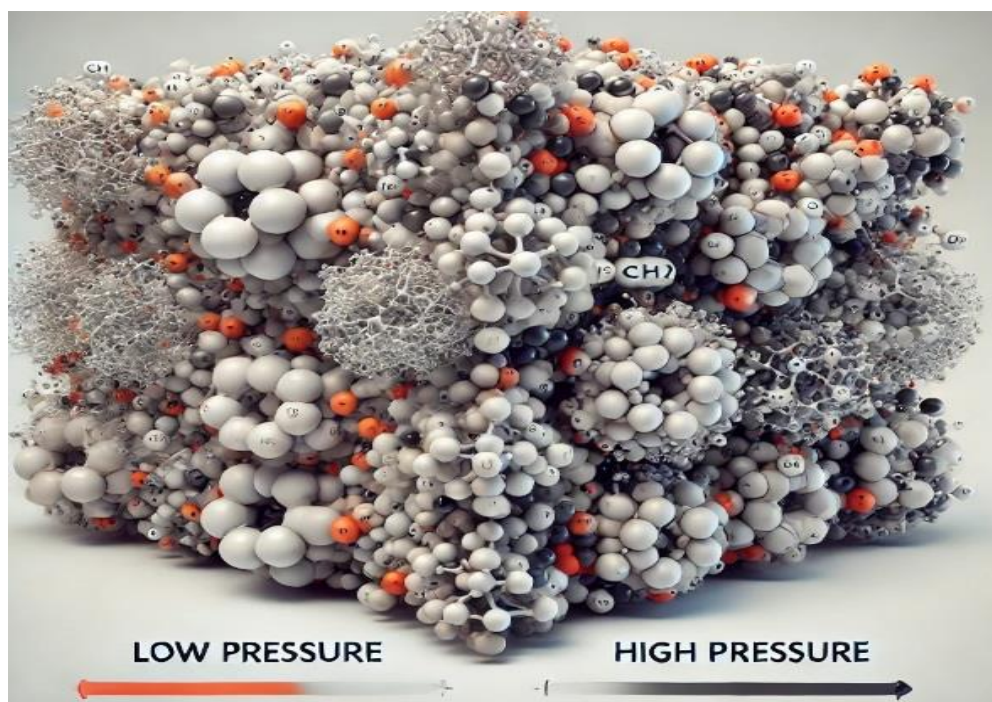


Figure 11 Phase transitions by pressure variations

- **Left side (low pressure):** Disordered, amorphous arrangement with significant spacing between atoms.
- **Right side (high pressure):** Densely packed, aligned, and semi-crystalline structure

Thus plastics can be degraded or altered through **temperature and pressure variations**, but the extent and nature of degradation depend on the type of plastic and the conditions applied. Here's how temperature and pressure affect the degradation or transformation of plastics:

11. Conclusion

The analysis and comparative study of phase transitions of different types of plastic waste under varying pressure conditions provide critical insights into their thermal and mechanical behavior. This research highlights the distinct phase transition characteristics of each plastic type, influenced by their chemical composition and structural properties. The results emphasize the importance of pressure as a significant factor in modulating the thermal properties and phase stability of plastics. Understanding these transitions can inform the development of optimized recycling processes, improved material recovery techniques, and sustainable waste management strategies. Additionally, the study underscores the potential for tailoring pressure and temperature conditions to enhance the efficiency of recycling methods and reduce the environmental impact of plastic waste.

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