X-ray analysis for quantifying various components in poly(vinyl chloride) plastics

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Poly(vinyl chloride), a.k.a. PVC, is a common plastic of everyday life found in products such as water piping, construction materials, medical applications, automotive parts, and consumer goods (furniture, clothing, sports equipment, etc…)[1]. The annual worldwide production of this commodity plastic reached 39 million tons in 2013 and is second in commercial production only to polyethylene[2]. To improve the plastic performance, adapt it to its various uses and control costs, components such as thermal stabilizers (tin based), lubricants (such as calcium stearate $(C_{18}H_{35}O_2)_2Ca.H_2O$), pigments ($TiO_2$), and filler ($CaCO_3$) are added to the PVC resin. The complexity of these formulations commonly leads to deposition of materials near the die extrusion orifice typically referred to as "plate out materials". Understanding the nature and composition of these deposits, but also of the PVC plastic formulation itself, is of great help to the plastic extruder and formulator in minimizing this issue, especially considering that plate out formation eventually leads to extrusion line shutdown for cleaning and lost production time. Materials identified in plate out naturally correspond to those found in the parent PVC formulation along with possible degradation products. Elemental analysis with X-ray fluorescence is a useful approach to obtain concentration levels of the various components from the initial PVC formulation or the plate out material, but is not sufficient in all cases. Since both calcium stearate (lubrication) and calcium carbonate (filler) are used in PVC formulation, X-ray diffraction is also used in this study to identify and quantify them individually. The few investigations conducted on calcium stearate have shown stronger diffracted intensities in the low angle region (corresponding to the stacking of two calcium stearate molecules) and temperature effects on polymorphism[3,4]. A monoclinic cell has also been proposed to explain most of calcium stearate observed reflections[5]. Using literature information and reference data we focused on using X-ray diffraction analysis to quantify these two classes of calcium compounds along with other phases present in PVC plastics and in plate out materials.

References

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